CHEMICAL ENGINEERING TRANSACTIONS

VOL. 31, 2013

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet

Guest Editors: Eddy De Rademaeker, Bruno Fabiano, Simberto Senni Buratti

ISBN 978-88-95608-22-8; **ISSN** 1974-9791

DOI: 10.3303/CET1331122

CFD Simulations of the Effect of Dust Diameter on the Dispersion in the 20 L Bomb

Valeria Di Sarli[a], Paola Russo[b], Roberto Sanchirico[a], Almerinda Di Benedetto*[c]

[a]Istituto di Ricerche sulla Combustione, CNR, Via Diocleziano 328, 80124, Napoli (IT)
[b]Dipartimento di Ingegneria Industriale, Università di Salerno, via Ponte don Melillo, 84084 Fisciano Salerno (IT)
[c]Dipartimento di Ingegneria Chimica, Università degli Studi “Federico II”, Piazzale Tecchio 80, 80125, Napoli (IT)
almerinda.dibenedetto@unina.it

Prevention and mitigation measures for dust explosion are based on the knowledge of the thermo-kinetic parameters which characterise flammability such as Minimum Explosible Concentration, MEC, and explosion behaviour such as maximum explosion pressure, P_{MAX}, and deflagration index, K_{St}.
Measurements of these parameters are performed in spherical vessels (20 L sphere or 1 m^3 sphere). The main issues in performing such measurements are related to the dust dispersion and to the turbulence level reached inside the sphere.
Also, the dispersion and then concentration of the dust/air mixture in the vessel significantly affects the flame propagation, if stratification and sedimentation occurs.
In this work we use a previously validated CFD 3D model to simulate the dust dispersion inside the sphere at different dust diameters. Results show that on increasing the dust diameter the dust is mainly concentrated at the vessel walls and the dust paths are different from those of the fluid flow.

1. Introduction

In chemical processes (food, pharmaceutical and wood industries, chemical manufacturing), a high number of accidents are imputable to explosions of flammable dusts causing failure to equipment, injuries and damages to people and surrounding environment.
Prevention and mitigation measures are based on the knowledge of the thermo-kinetic parameters which characterize the flammability (Minimum Ignition Energy, MIE; Minimum Ignition Temperature, MIT; Minimum Explosible Concentration, MEC; Limiting Oxygen Concentration, LOC) and explosion (Maximum Explosion Pressure, P_{MAX}; Deflagration Index, K_{St}) of dust/air and/or dust-gas/air mixtures.
The evaluation of these parameters may be performed both experimentally (Eckhoff, 2003) and theoretically by modelling the dust explosion as explosion of the pyrolysis products (Di Benedetto and Russo, 2007) also taking into account the effect of the dust size (Di Benedetto et al., 2010). Recently, Dufud et al. (2012) confirmed the relevant role of the pyrolysis step in the modelling of explosion of organic dusts.
Experimental tests are performed according to well established standard procedures (Eckhoff, 2006).
In the case of the evaluation of P_{MAX}, K_{St} and MEC tests are performed in a spherical vessel (20 L sphere and/or 1 m^3 sphere).
The procedure is based on injecting the dust in the sphere, initially pre-evacuated at 0.4 bar, through a valve connecting a container loaded with dust and pressurized with 21 bar of compressed air. At the bottom side of the bomb, in the 20 L sphere a rebound nozzle is placed to allow dispersion of the dust/air mixture inside the vessel. The most relevant issue of this procedure is the dust dispersion inside the bomb which should ensure a uniform dust concentration.
In a previous paper (Di Sarli et al., 2012), we developed a three-dimensional CFD model to describe the turbulent flow field induced by dust feeding and dispersion within the 20 L bomb and the associated effects on the distribution of dust concentration.

Please cite this article as: Di Sarli V., Russo P., Sanchirico R. and Di Benedetto A., 2013, Cfd simulations of the effect of dust diameter on the dispersion in the 20 l bomb, Chemical Engineering Transactions, 31, 727-732 DOI: 10.3303/CET1331122

The developed CFD model has been successfully validated against measurements of time histories of pressure and root mean square velocity available in the literature. The model results show the presence of multiple turbulent vortex structures which generate dead volumes for the dust, pushed toward the walls of the sphere. The dust concentration was found as not uniform in the sphere, being higher close to the vessel walls and much lower than the nominal value. In this work we extend our model to simulate the effect of dust size on the dust dispersion.

2. Model description

Model details are given elsewhere (Di Sarli et al., 2012). Briefly, it consists on the time-averaged Navier-Stokes equations (Eulerian approach) written in polar coordinates. The numerical simulation of the turbulence was performed by using the standard k-ε model (Launder and Spalding, 1972).

The flow of the solid phase was solved with the Lagrangian approach using the Discrete Phase Model (DPM).

The interaction between the fluid phase and the solid particles was assumed as two-way since according to the classification of Elghobashi (1994), the operating conditions (particle volume fraction, particle density and particle concentration) suggest that the fluid flow affects the particle motion and vice versa, while the particle-particle collisions (which are accounted for in the four-way coupling) may be neglected.

The fluid flow equations were discretized using a finite-volume formulation on the three-dimensional non-uniform unstructured grid (total cell number 1016951). The spatial discretization of the model equations used first order schemes for convective terms and second order schemes for diffusion terms. First-order time integration was used to discretize temporal derivatives with a time step of $1 \cdot 10^{-4}$ s.

Parallel calculations were performed by means of the segregated pressure-based solver of the code ANSYS Fluent (release 14).

The Discrete Phase Model was described by ordinary differential equations (on the contrary, the continuous flow was described by partial differential equations). Therefore, the DPM used its own numerical mechanisms and discretization schemes. For particle tracking, we used an automated scheme which provides a mechanism to switch in an automated fashion between numerically stable lower order schemes and higher order schemes, which are stable only in a limited range. In situations where the particle is far from hydrodynamic equilibrium, an accurate solution can be achieved very quickly with a higher order scheme. When the particle reaches hydrodynamic equilibrium, the higher order schemes become inefficient and the mechanism switches to a stable lower order scheme. We choose the Euler integration as lower order scheme and the semi-implicit trapezoidal integration as higher order scheme. The particle tracking integration time step was taken equal to the fluid flow time step ($1 \cdot 10^{-4}$ s).

The simulation conditions are summarised in Table 1.

Table 1: Simulation conditions

Dust Container vessel volume (L)	0.6
Sphere Volume (L)	20
Initial pressure of container (bar)	21
Initial pressure of sphere (bar)	0.4
Dust density (kg/m^3)	2046
Dust diameter (μm)	10
Dust concentration (g/m^3)	250

3. Results

The velocity vectors in the central section of the sphere coloured by the dimensionless dust concentration $\gamma = C/C_{nominal}$ as obtained at d = 10 μm (Figure 1), at d = 100 μm (Figure 2) and at d = 250 μm (Figure 3) are shown. In Figure 1 it is noting the presence of two main vortices in the central plane which generate dead volumes. Coherently, the dust concentration is very low in the vortex cores while it increases on the outer zone of the vortices. It is noting that dust particles are partially entrained by the fluid flow.

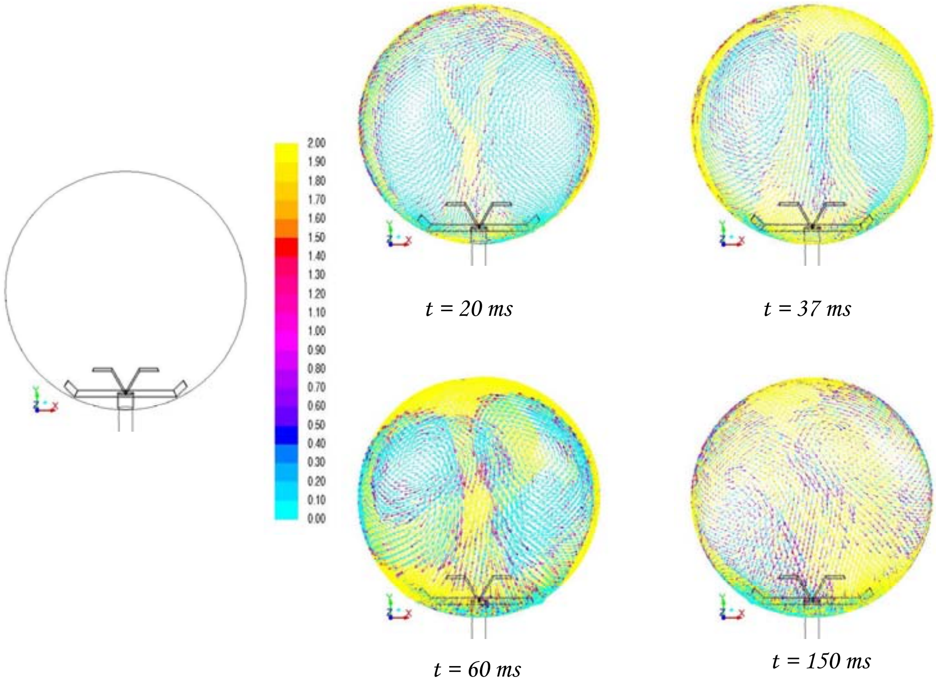

Figure 1: The velocity vectors in the central section of the sphere coloured by the dimensionless dust concentration $\gamma = C/C_{nominal}$ as obtained at $d = 10\ \mu m$ $C = 250\ g/m^3$

On increasing the dust diameter (Figure 2 and 3), it becomes more difficult for the fluid flow to entrain the dust which then follows a completely different path with respect to the fluid.

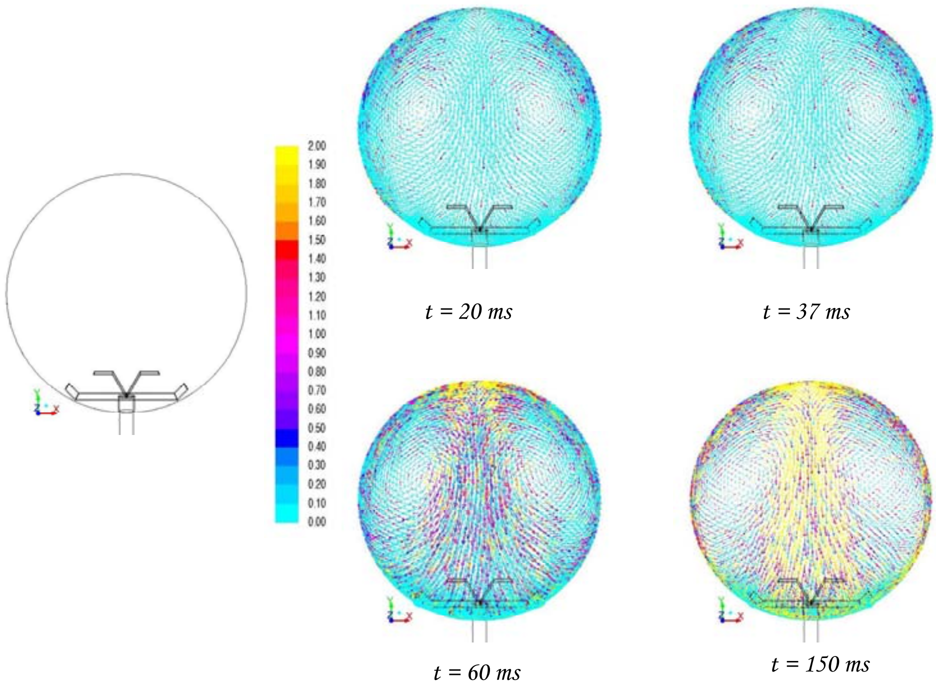

Figure 2: Velocity vectors in the central section of the sphere coloured by the dimensionless dust concentration $\gamma = C/C_{nominal}$ as obtained at $d = 100\ \mu m$ and $C = 250\ g/m^3$.

In order to better visualise the preferential paths of the dust, we mapped the particle tracks. In Figures 4-6 the particle tracks at different time instants are shown as coloured by the dimensionless dust concentration $\gamma = C/C_{nominal}$ as obtained at d = 10 μm (Figure 4), at d = 100 μm (Figure 5) and at d = 250 μm (Figure 6).

It is found that the dust has preferential paths which are determined by the vortices generate in the sphere after the dust injection from the container (Di Sarli et al., 2012). After the ignition time (t_v = 60 ms), the dust is mainly concentrated on the vessel wall. On increasing the dust diameter the preferential paths are much more evident suggesting that the dust dispersion is worst and worst.

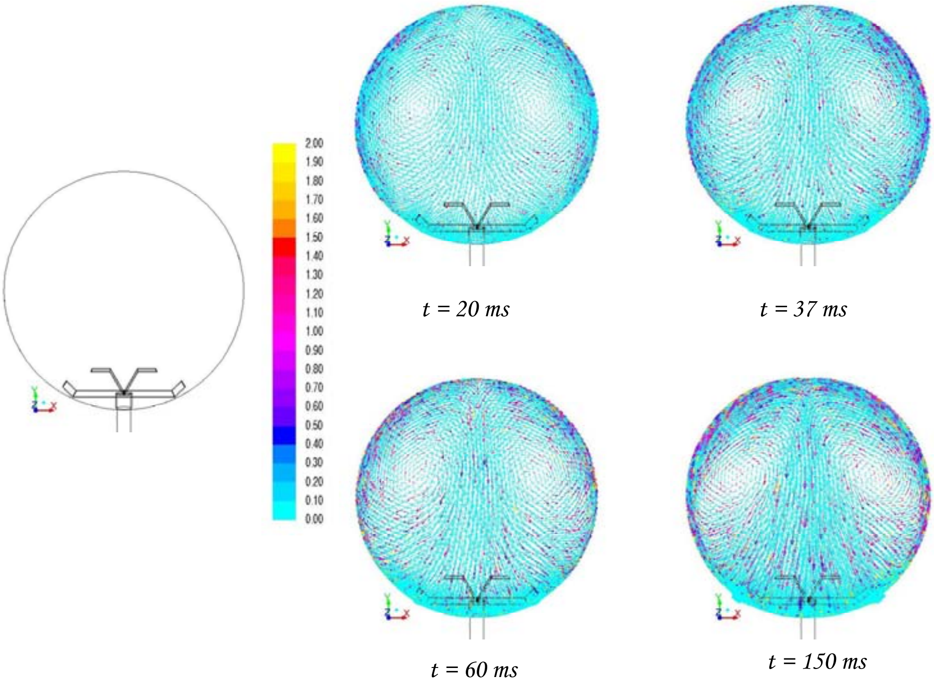

Figure 3: Velocity vectors in the central section of the sphere coloured by the dimensionless dust concentration $\gamma = C/C_{nominal}$ as obtained at d = 250 μm and C = 250 g/m^3.

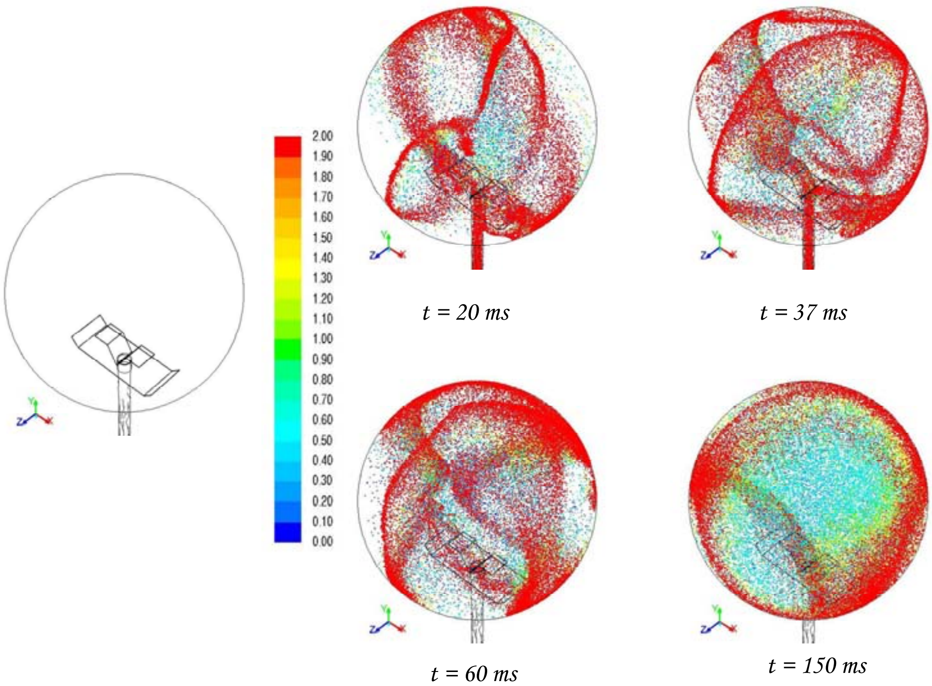

Figure 4: Particle tracks coloured by the dimensionless dust concentration at dust diameter d = 10 μm and C = 250 g/m^3.

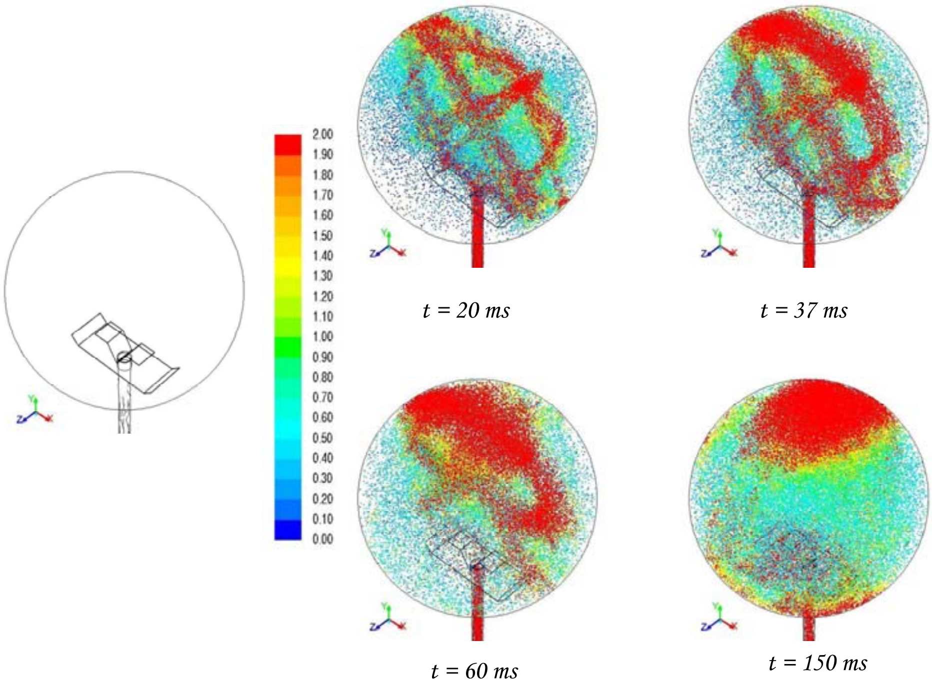

Figure 5: Particle tracks coloured by the dimensionless dust concentration at dust diameter d = 100 μm and C = 250 g/m^3.

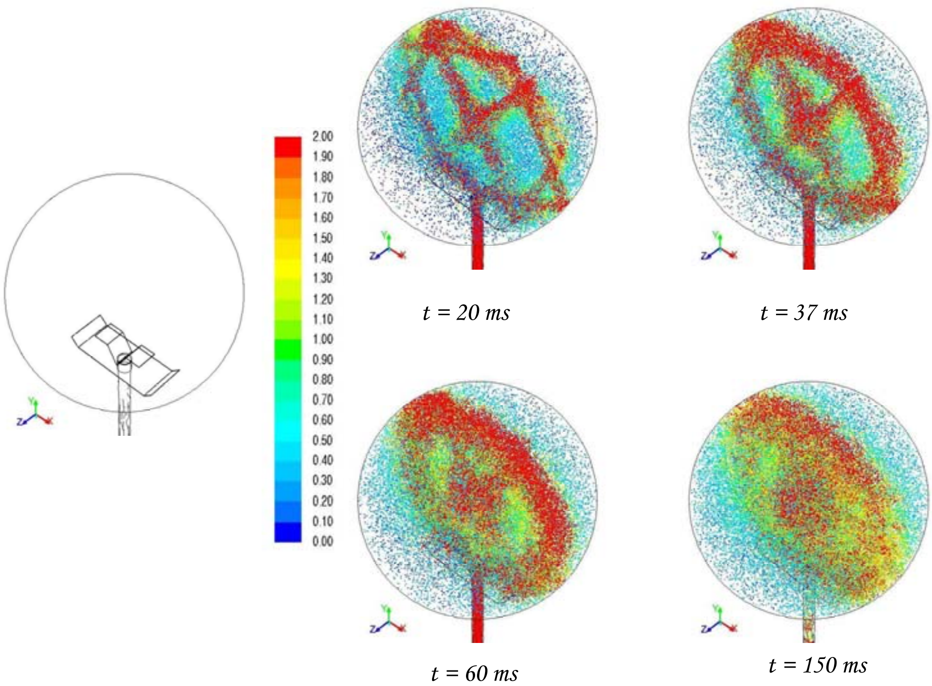

Figure 6: Particle tracks coloured by the dimensionless dust concentration at dust diameter d = 250 μm and C = 250 g/m^3.

The results here obtained suggest that the dust concentration is completely different from the nominal value. For practical applications, this deviation may not be relevant when measuring the maximum K_{St} values at varying the nominal dust concentration, but is not allowed when measuring the minimum explosive concentration (MEC). As a consequence, different methods for measurement of MEC a different method of dust dispersion is needed.

4. Conclusions

A three-dimensional CFD model previously validated was used to simulate the dust dispersion inside the 20 L bomb at different values of the dust diameter.
The time sequences of velocity vector maps show that multiple turbulent vortex structures are established within the sphere, generating dead volumes for the dust which is pushed toward the walls of the sphere.
At low values of the dust diameter (d = 10 μm), the dust is partially entrained by the fluid filling the outer region of the vortex and partially the internal zones.
On increasing the dust diameter (d = 100 μm and d = 250 μm) the dust and the fluid flows are independent and the dust follows flow paths completely different being concentrated mainly at the vessel walls.
The results here obtained suggest that a different dust dispersion method has to be developed mainly for the measurement of the minimum explosive concentration, MEC.

References

Code ANSYS FLUENT, www.ansys.com.
Di Benedetto A, Russo P. Thermo-kinetic modelling of dust explosions. Journal of Loss Prevention in the Process Industries. 2007; 20: 303-309.
Di Benedetto A, Russo P, Amyotte PR, Marchand N. Modelling the effect of particle size on dust explosions. Chemical Engineering Science. 2010; 65: 771-779.
Di Benedetto A., Russo P., Sanchirico R., Di Sarli V.CFD simulations of turbulent fluid flow and dust dispersion in the 20 liter explosion vessel2012 AIChE J, in press.
Dufaud O., Khalili I., Cuervo N., Olcese R., Dufour A., Perrin L., Laurent A., Highlighting the Importance of the Pyrolysis Step on Dust Explosions, Chemical Engineering Transactions (2013); 26 369-374
Eckhoff RK. Explosions in the Process Industries (3rd edition). Gulf Professional Publishing, 2003.
Eckhoff RK. Differences and similarities of gas and dust explosions: A critical evaluation of the European 'ATEX' directives in relation to dusts. Journal of Loss Prevention in the Process Industries. 2006; 19: 553-560.
Elghobashi S. On predicting particle-laden turbulent flows. Applied Scientific Research. 1994; 52: 309-329.
Launder BE, Spalding DB. Lectures in Mathematical Models of Turbulence. Academic Press, London, United Kindom, 1972.