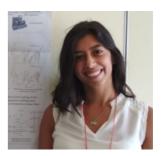
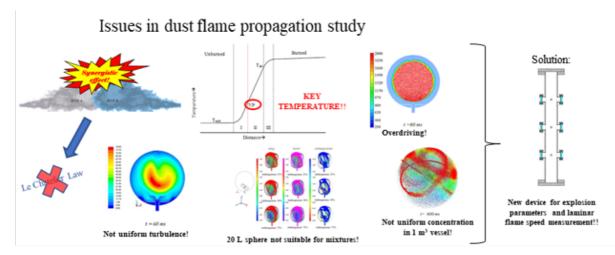
## TURBULENT FLAME PROPAGATION OF DUSTS AND DUST MIXTURES



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In chemical processes, several accidents are imputable to explosions of combustible dusts, dust mixtures, and hybrid mixtures. To characterize the sensitivity and the severity of explosion in case of ignition, the explosibility and flammability parameter assessment is required. Most of these parameters are measured in 20 L and/or 1 m<sup>3</sup> vessels, according to standard procedures. There are at least two main requirements for repeatable and reliable measurements of flammability and explosibility parameters of dusts: a uniform dispersion of solid particles inside the test vessel and a homogeneous degree of turbulence. In the literature, it has been shown that in the standard 20 L sphere these requisites are not satisfied. It is not clear how the 1 m<sup>3</sup> vessel performs. These conditions significantly affect the explosion parameters since they have a direct role in driving the unsteady flame propagation.

This PhD thesis aims at designing and developing a novel equipment able to produce reliable and repeatable measurements of the explosion/flammability parameters. To this end, control of particle dispersion and concentration and turbulence level is required. The main focus is the identification of the mechanisms affecting the explosion features and then the flame propagation by means of both an extensive experimental and modeling approach.

The first year of the PhD was primarily focused on the study and characterization of the thermal behavior of dusts and dust mixtures to gain insight into their physicochemical transformation during ignition and flame propagation. Depending on the mixtures, a synergistic behavior has been found between the pure dusts constituting the mixture due to physical and/or chemical reactions. For some mixtures, the more severe behavior has been attributed to the presence of a eutectic point (niacin/ anthraquinone, ascorbic acid/niacin), in other cases, to chemical reactions with the formation of volatiles (ascorbic acid/irganox 1222, ascorbic acid/glucose). On this basis, we propose a new classification of dusts mixtures in three mixtures safety classes (MSC)<sup>1,2</sup>.

In the second and third years a detailed analysis of the main issues of the standard equipment (20 L and  $1 \text{ m}^3$ ) has been performed by developing a CFD able to simulate the dust dispersion within both vessels equipped with the perforated annular nozzle or the rebound one. The models previously validated against the available experimental data, were used to simulate the spatial/temporal evolution of dust concentration and turbulent flow in both vessels.

Results showed that the initial turbulence level established in the 20 L vessel is always higher than that found in the  $1 \text{ m}^3$  vessel. In the 20 L vessel a high dispersion of the dust concentration is obtained while in the  $1 \text{ m}^3$  a quite uniform turbulence level is achieved. In both the standard vessel, the requirement of a uniform dust cloud within the test

volume is not satisfied. In particular, the highest dust concentrations are attained externally to the vortices, whereas the dust concentration is very low inside the vortices <sup>3,4,5</sup>.

Starting from these results, the effect of the initial turbulence level on the most important explosion parameter, deflagration index ( $K_{st}$ ) was assessed. Calculations showed that in the 20 L vessel  $K_{st}$  is always higher with respect to that evaluated in the 1 m<sup>3</sup> vessel and more dependent from the dust properties (diameter, density, and shape). As a main conclusion, the difference between the explosion tests in the 20 L and 1 m<sup>3</sup> vessels, are qualitative other than quantitative being not only the turbulent kinetic energy different but also the turbulent combustion regime (thin reaction zone and corrugated flamelets for 20 L and 1 m<sup>3</sup> respectively) which significantly affects the flame propagation mode and eventually the explosion severity <sup>6</sup>.

The role of the pyrotechnic ignitors on the pressure trend and the temperature distribution was also tested in both vessels. Results showed that the flame propagation generated by the ignitors is very relevant in the 20 L sphere leading to the overdriving phenomenon. CFD simulations show that the hot core generated by the ignitors dissipate much faster in the 20 L vessel than in the 1 m<sup>3</sup> vessel, due to the higher turbulence level of the smaller vessel. Therefore, dusts whose combustion is controlled by particle heating are more prone to sustain combustion in the 1 m<sup>3</sup> than in the 20 L vessel <sup>7</sup>.

All the obtained results allowed to design a novel equipment, theoretically able to produce reliable and repeatable measurements of the explosion/flammability parameters. Fluid dynamics studies of the novel equipment are currently underway thanks to the use of CFD models and the development of a twin equipment in polycarbonate.

## **References:**

- 1. Centrella, L., <u>Portarapillo, M.\*</u>, Luciani, G., Sanchirico, R., Di Benedetto, A. Synergistic behavior of flammable dust mixtures: A novel classification, Journal of Hazardous Materials, 397, 122784, 2020 DOI: <u>https://doi.org/10.1016/j.jhazmat.2020</u>
- Portarapillo, M., Luciani, G., Sanchirico, R., Di Benedetto, A. Ignition mechanism of flammable dust and dust mixtures: an insight through TG / DSC analysis, AIChE Journal, e16256, 2020 DOI: <u>https://doi.org/10.1002/aic.16256</u>
- 3. <u>Portarapillo, M.</u>, Di Sarli, V., Sanchirico, R., Di Benedetto, A. CFD Simulation of the Dispersion of Binary Dust Mixtures in the 20 L Vessel, Journal of Loss Prevention in the Process Industries, 67, 104231, 2020, DOI: <u>https://doi.org/10.1016/j.jlp.2020.104231</u>
- 4. <u>Portarapillo, M.</u>, Trofa, M., Sanchirico, R., Di Benedetto, A. CFD Simulations of Dust Dispersion in the 1 m<sup>3</sup> Explosion Vessel, Journal of Loss Prevention in the Process Industries, 68, 104274, 2020, DOI: <u>https://doi.org/10.1016/j.jlp.2020.104274</u>
- 5. <u>Portarapillo, M.</u>, Trofa, M., Sanchirico, R., Di Benedetto, A. CFD simulations of the effect of dust diameter on the dispersion in the 1 m<sup>3</sup> explosion vessel, Chemical Engineering Transaction, 86, 2021
- Portarapillo, M.\*, Sanchirico, R., Di Benedetto, A. Effect of turbulence spatial distribution on the deflagration index: Comparison between 20 L and 1 m<sup>3</sup> vessels, Journal of Loss Prevention in the Process Industries, 71, 104484, 2021, DOI: <a href="https://doi.org/10.1016/j.jlp.2021.104484">https://doi.org/10.1016/j.jlp.2021.104484</a>
- Portarapillo, M., Sanchirico, R., Di Benedetto, A. On the pyrotechnic ignitors role in dust explosion testing: Comparison between 20 L and 1 m<sup>3</sup> explosion vessels, Process Safety Progress, e12249, 2021, DOI: <u>https://doi.org/10.1002/prs.12249</u>

## Additional papers:

- <u>Portarapillo, M.</u>, Aronne, A., Di Benedetto, A., Landi, G., Luciani, G. Syngas production through H<sub>2</sub>O/CO<sub>2</sub> thermochemical splitting, Chemical Engineering Transaction, 74, 43-48, 2019 DOI: <u>https://doi.org/10.3303/CET1974008</u>
- <u>Portarapillo, M.</u>, Muscetta, M., Di Benedetto, A., Andreozzi, R. Risk Analysis of Sodium Hypochlorite Production Process, Chemical Engineering Transaction, 82, 49-54, 2020, DOI: <u>https://doi.org/10.3303/CET2082009</u>
- <u>Portarapillo, M.\*</u>, Di Benedetto, A. Risk Assessment of the Large-Scale Hydrogen Storage in Salt Caverns, Energies, 14 (10), 2856, 2021, DOI: <u>https://doi.org/10.3390/en14102856</u>
- Danzi, E., Di Benedetto, A., Sanchirico, R., <u>Portarapillo, M.</u>, Marmo, L. Biomass from Winery Waste: Evaluation of Dust Explosion Hazards, Chemical Engineering Transaction, 86, 2021