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Review of a Dust Explosion Modeling

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A single particle model developed for dust explosion is here reviewed. The model describes the behaviour of a reacting particle which undergoes different steps during reaction: heating, devolatilization and homogeneous combustion. The model predicts the maximum values of the deflagration index, also including the role of turbulence. Four explosion regimes have been introduced to take into account the effect on the K_{St} value of the dust diameter and of the dust shape (different from sphere). These regimes are defined as function of dimensionless numbers (*Bi, Da, Th*) which contain the chemico-physical properties of the dust-air mixtures. The effect of fuel gas addition to dust was also included in the model by calculating an equivalent gas mixture composition given by the flammable gas present in the hybrid mixture and the pyrolysis products generated from the dust pyrolysis.
Finally, a guideline for the dust explosion simulations is proposed and modeling perspective discussed.

1. Introduction

Modelling dust explosion is still a scientific challenge. Different scales of model for dust explosion are involved: large scale where the dust-air flame propagation is simulated for computing the overpressure, down to the single particle model used to evaluate the most important thermo-physical parameters like the burning velocity, the deflagration index, the minimum ignition temperature.
The simulation of the unsteady flame propagation of a dust in large scale requires the evaluation of the intrinsic reactivity of the dust-air mixture and the coupling between combustion and turbulent fluid flow.
In literature attempts for modeling dust esplosion are present mainly based on the CFD approaches (Skjold, 2007; Skjold et al., 2008). In these models the dust-air flame is treated as a gas-air flame and the dust thermo-physical properties are derived from parallel experiments. At the moment, hence, the two-phase modeling of the dust-air flame propagation and its coupling with turbulence is an open issue.
At the particle scale, several models (Continillo, 1989; Callè et al., 2005; Di Benedetto and Russo, 2007a) have been proposed for the evaluation of the thermo-physical properties as a promising alternative to experiments which are strongly affected by dust dispersion degree, initial turbulence level, particle size distribution (Cashdollar, 2000; Eckhoff, 2003).
In the model of Continillo et al. (1989) the laminar flame propagation through a coal dust/air mixture in a explosion vessel was evaluated by assuming single particle explosion. The pyrolysis rate of particle as well as the combustion of volatiles are modeled as a one-step Arrhenius reaction.
Callè et al. (2005) proposed a single particle model of cellulose dust where the reaction is assumed to proceed mainly via a single heterogeneous step.
More recently, Di Benedetto and Russo (2007a) and Di Benedetto et al. (2010a) developed a single particle model able to describe the reacting particle which undergoes different steps during reaction: heating, heterogeneous combustion, devolatilization and homogeneous combustion; all of them strongly influenced by dust properties (i.e. mean particle diameter). In these models the combustion of volatiles is described by means of a detailed reaction mechanism (53 species and 325 elementary steps).
We also extended the model to take into account the effect of the dust shape (Russo et al., 2012a) and of adding flammable gas (Russo et al., 2012b).

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In this review we propose a guideline for the dust explosion simulations also discussing the modeling perspective.

2. Thermokinetic modelling

The main step through which a single particle reacts are schematized in figure 1. The dust particle is heated, producing volatiles which may react with the air, then producing heat. Parallely, the dust particle may react directly with oxygen diffusing towards the particle itself.

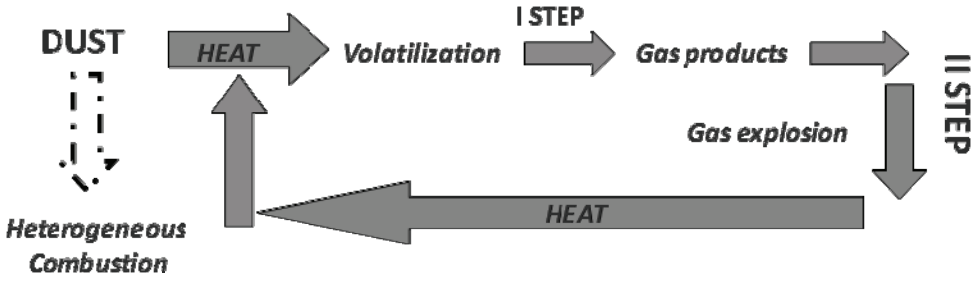

Figure 1: Schematic representation of dust explosion path .

The most important parameter affecting the relevance of each step with respect to the other is the dust size. At values of the diameter lower than a critical value (Cashdollar et al., 1989; Eckhoff, 2003), the dust explosion is mainly controlled by homogeneous combustion.
We have developed a model of dust explosion based on a detailed reaction mechanism assuming that the pyrolysis/devolatilization step is very fast and gas combustion is controlling dust explosion (Di Benedetto and Russo, 2007a). The model consists on 3 modules. The first one simulates the flame propagation to evaluating the laminar burning velocity, S_l. The second one allows the evaluation of the adiabatic pressure (P_{max}) and the third one of the maximum pressure rise (dP/dt_{max}) and deflagration index (K_{St}). The homogeneous combustion of the gas volatiles was simulated by using the GRI-Mech3.4 detailed reaction mechanism, implemented in the CHEMKIN module to calculate the laminar burning. The deflagration index was calculated by the cubic law here reported:

$$K_{St} = \left(\frac{dP}{dt}\right)_{max} V^{1/3} \tag{1}$$

where the maximum pressure rise is calculated according to the formula:

$$\left(\frac{dP}{dt}\right)_{max} = \frac{3\left(P_{max} - P_0\right)}{R_{vessel}}\left[1 - \left(\frac{P_0}{P}\right)^{\frac{1}{\gamma}} \frac{P_{max} - P}{P_{max} - P_0}\right]^{\frac{2}{3}} \left(\frac{P}{P_0}\right)^{\frac{1}{\gamma}} S_l \tag{2}$$

where P_{max} is the maximum pressure reached in a closed vessel obtained by using the equilibrium module of the CHEMKIN code. R_{vessel} is the radius of the reference spherical vessel (20 L) and Po is the initial pressure (1 bar).
The deflagration index, maximum pressure and burning velocity calculated, valid for very low values of the dust size, have to be considered as asymptotic values.
We computed the laminar burning velocity, the maximum pressure and then the deflagration index for corn starch, cellulose and polyethylene and we successfully compared them with experimental values (Table 1).

Table 1: Comparison between K_{St} values from model and experiments

Dust	K_{St} Model	K_{St} Experimental	Error (%)
Corn Starch	204	200	2
Cellulose	140	126	11
Polyethylene	211	203	4

The model above described has been recently extended to calculate the minimum ignition temperature (MIT) (Di Benedetto et al., 2010b). The theoretical evaluation was performed at varying the residence time and the dust concentration and an asymptotic value was found for each concentration. MIT values are measured using the Godbert-Greenwald furnace where the residence time and the dust concentration are not univocally set. Typically, the lowest value of a grid of results is assumed as the most conservative value. The comparison between computed and experimental data of MIT of polyethylene shows that the model is able to predict the value with good agreement with the experimental ones.

3. Effect of the dust size

For the simulation of explosion of dust particles with size larger than the critical value, the model was extended to include devolatilization rate and particle heating (Amyotte et al., 2010; Di Benedetto et al., 2010a). The model solves the energy and mass balances of the single particle and the gas phase coupled to the combustion reaction rate. The model results were successfully compared to the experimental data from polyethylene explosion tests (Di Benedetto et al., 2010a).
From the model results we also defined four explosion regimes which take into account the effect of the dust size on the K_{St} value as function of dimensionless numbers which contain the chemico-physical properties of the dust-air mixtures (i.e., Biot number that is measure of the internal heat conduction time with respect to the external heat transfer time).
For *Bi*«1 the characteristic times of external heat transfer (the slowest process) should be compared with the characteristic reaction time. This is usually done through the Damkohler number:

$$Da = \frac{t_e}{t_{pyro}} = \frac{r_p \Delta T_i c_p d}{h_c \Delta T_i + \varepsilon \sigma \Delta T_i^4} \tag{3}$$

Two regimes can be observed:

- Regime I (*Bi*«1 and *Da*»1): when conversion occurs under the external heat transfer control;
- Regime II (*Bi*«1 and *Da*«1): when conversion occurs under the control of the pyrolysis chemical reaction.

For *Bi*»1, the characteristic time associated with internal heat transfer (the slowest process) should be compared with the characteristic time of pyrolysis chemical reaction. This is done by means of the thermal Thiele number:

$$Th = \frac{t_c}{t_{pyro}} = \frac{r_p c_p d^2}{\lambda} \tag{4}$$

Thus, for *Bi*»1, two regimes can be observed:

- Regime III (*Bi*»1 and *Th*«1): when conversion occurs under the pyrolysis chemical kinetic control;
- Regime IV (*Bi*»1 and *Th*»1): when conversion occurs under the control of internal heat transfer.

In each regime we computed the module χ defined as the ratio between the deflagration index at diameter d and the asymptotic value of the deflagration index ($K°_{St}$):

$$\chi(d) = \frac{K_{St}(d)}{K_{St}^0} \tag{5}$$

In Figure 2 the χ module is plotted versus the dust diameter as obtained in the four regimes identified (lines), toghether with the experimental values (symbols).
The diagram of figure 2 can be easly used through the following steps:

- Evaluation of the dimensionless numbers and then of the explosion regime (I, II, III or IV);
- Evaluation of the asymptotic K_{St} value through the model of Di Benedetto and Russo (2007a);
- Enter into the diagram for evaluating the χ module and then the final K_{St} value.

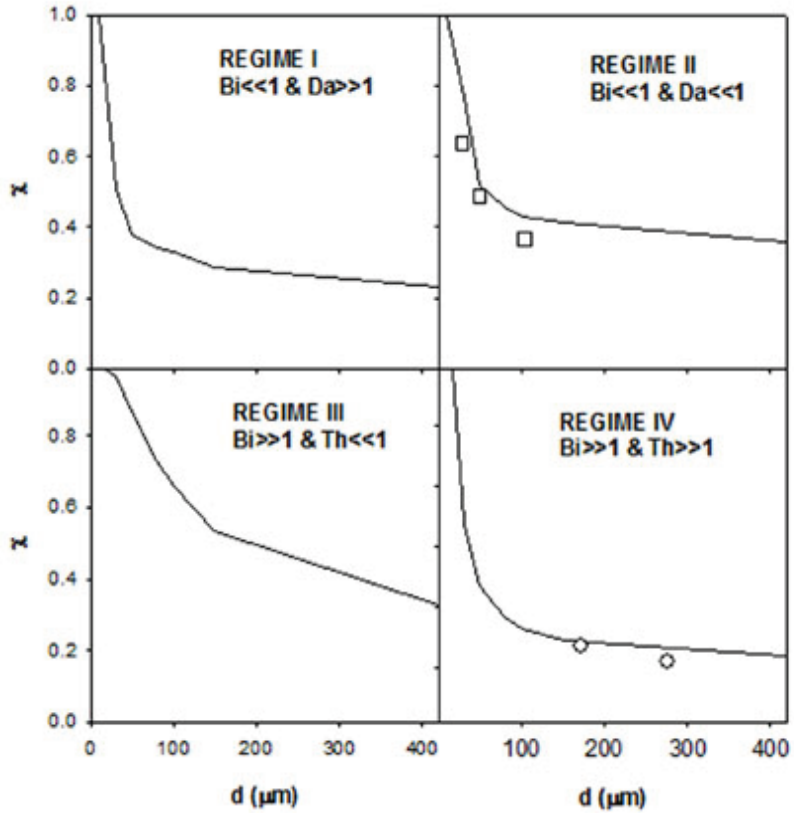

Figure 2. Explosion regimes diagram for taking into account the effect of the dust diameter.

4. Effect of the dust shape

The model above described was developed for spherical particles. Actually, in many applications the dusts have a fiber nature showing a cylindrical shape with very high length to diameter ratio. Fibrous materials may either be natural (i.e. wool, cellulose) or synthetic (i.e. nylon). Ignitability and explosibility of synthetic flock materials were discussed recently by Marmo and Cavallero (2008), Worsfold et al. (2012) and Salatino et al. (2012).

We recently extended our previous model to dust with cylindrical shape. To this end, we calculated a characteristic size of the flock, D_{eq} as follows:

$$D_{eq} = 2\sqrt{\frac{d_f L}{\pi}} \tag{6}$$

where d_f is the diameter and L is the length of flock. The equivalent diameter, D_{eq}, is the diameter of a sphere having the area equal to that of the fibre (cylinder). Then, the procedure described above can be applied to determine the deflagration index of flocculent materials as a function of the equivalent diameter.

We used the model for nylon dust of cylindrical shape with d_f = 11-50 μm and L = 0.3-1 mm (Iarossi et al., 2012). We found that this dust explodes in regime III up to D_{eq} = 130 μm and in regime II for D_{eq}>130 μm (Russo et al., 2012a). In figure 3 the experimental and theoretical values of K_{St} are shown. The agreement is quite good. These results can not be generalized to all fibers since they have been validated only for low values of d_f/L (0.02 - 0.06).

Future studies should be focused on the evaluation of the critical d_f/L ratio for which the dust explosion behavior can be described with this model.

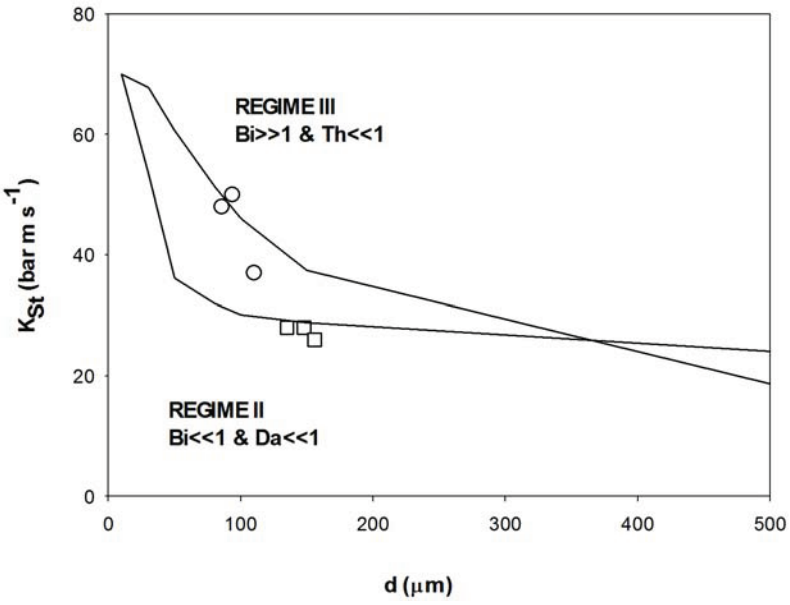

Figure 3. K_{St} as function of the nylon D_{eq} as computed by the model (lines) and by experiments (symbols).

5. Hybrid mixture models

Another important research field is the modeling of hybrid (dust+gas/air) mixtures.
We proposed a model for describing the effect of fuel gas addition to the dust by calculating an equivalent gas mixture composition given by the flammable gas present in the hybrid mixture and the pyrolysis products generated from the dust pyrolysis (Amyotte et al., 2010). We used this approach for computing the deflagration index for dust/gas-air mixtures at varying the fuel and dust concentration. The comparison with experimental data of hybrid mixture made of nicotin acid and methane was successful (Garcia Agreda et al., 2011; Russo et al., 2012b).
Future work should examine the effect of the dust diameter on deflagration index.

6. Effect of turbulence

In dust explosion tests, pre-ignition turbulence, necessary for suspending the dust clouds, has the feature of decaying in its intensity with time. The dust cloud is ignited at a defined delay time (60 ms) from the starting of dust dispersion and, hence, at a given initial level of turbulence.
To take into account this effect, the dependence of the deflagration index on the turbulence level was estimated by substituting in Eq. 2 the laminar burning velocity (S_l) with the turbulent burning velocity (S_t) as function of the velocity fluctuation (u') (Di Benedetto and Russo, 2007b). We used different formula available in literature for the evaluation of the turbulent burning velocity of both gas and dust. By comparing experimental and model results for corn starch and polyethylene we found that all the formula developed for gases give good prediction, while among the formula developed for dusts, the one proposed by Tezok et al. (1982) gives reasonable results.

7. Conclusions and future development

The model developed for dust explosion allows the evaluation of the maximum values of the deflagration index, also including the role of turbulence. The dust explosion regimes can be used for correcting the maximum values of the deflagration index when dust larger than the critical diameter are used and of different shape from spherical one.
In the future the model should be extended in order to take into account also the behavior of nano-particles which have size ranging from 1 to 100 nm. As recently reviewed by Worsfold et al. (2012) as particle size approaches the nanometer range the increase of the explosion severity is much less that that expected. This behavior has been related to two physical processes arising at nanosize: limited dispersibility and high coagulation rates. As a result of the incomplete dispersion and further coagulation, the effective size of particles will be greater than the particles' primary nanometer size. From these results it turns out that a novel model has to take into account dispersion degree and agglomeration.

References

Amyotte P., Lindsay M., Domaratzki R., Marchand N., Di Benedetto A., Russo P., 2010, Prevention and mitigation of dust and hybrid mixture explosions, Process Safety Progress 29 (1), 17-21.

Callé S., Klaba L., Thomas D., Perrin L., Dufaud O., 2005, Influence of the size distribution and concentration on wood dust explosion: Experiments and reaction modeling, Powder Technology 157, 144-148.

Cashdollar K.L., Hertzberg M., Zlochower I.A., 1989. Effect of volatility on dust flammability limits for coals, gilsonite, and polyethylene, in: Proceedings of the 22nd Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1757–1765.

Cashdollar K.L. , 2000, Overview of dust explosibility characteristics, Journal of Loss Prevention in the Process Industries 13, 183–199.

Continillo G., 1989, A two-zone model and a distributed-parameters model of dust explosions in closed vessels, Archivum Combustionis 9, 79–94.

Di Benedetto A., Russo P., 2007a, Thermo-kinetic modelling of dust explosions, Journal of Loss Prevention in the Process Industries 20 (4-6), 303-309.

Di Benedetto A., Russo, P., 2007b Model for the Evaluation of Thermo-kinetic Parameters of Dust Explosions, IChemE Symposium Series 153, 123/1-123/5.

Di Benedetto A., Russo P., Amyotte P., Marchand N., 2010a, Modelling the effect of particle size on dust explosions, Chemical Engineering Science 65 (2), 772-779.

Di Benedetto A., Di Sarli V., Russo P., 2010b, On the determination of the minimum ignition temperature for dust/air mixtures, Chemical Engineering Transactions 19, 189-194, DOI: 10.3303/CET1019031.

Eckhoff R.K, 2003, Dust Explosions in the Process Industries, Gulf Professional Publishing, USA.

Garcia-Agreda A., Di Benedetto A., Russo P., Salzano E., Sanchirico R., 2011, Dust/gas mixtures explosion regimes, Powder Technology 205 (1-3), 81-86.

Iarossi I., Amyotte P.R., Khan F.I., Marmo L., Dastidar A.G., Eckhoff R.K., 2012, Explosibility of polyamide and polyester fibers, IX ISHPMIE International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosions, 22-27 July 2012, Cracow, Poland, 21-1.

Marmo L., Cavallero D., 2008, Minimum ignition energy of nylon fibres, Journal of Loss Prevention in the Process Industries 17, 449-465.

Russo P, Amyotte P. R., Khan F. I., Di Benedetto A., 2012a, Modeling of the effect of size on flocculent dust explosions, IX ISHPMIE International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosions, 22-27 July 2012, Cracow, Poland, 12-3.

Russo P., Di Benedetto A., Sanchirico R., 2012b, Theoretical evaluation of the explosion regimes of hybrid mixtures, Chemical Engineering Transactions 26, 51-56, DOI: 10.3303/CET1226009.

Salatino P., Di Benedetto A., Chirone R., Salzano E., Sanchirico R., 2012, Analysis of an explosion in a wool-processing plant, Industrial & Engineering Chemistry Research 51 (22), 7713-7718.

Skjold T., 2007, Review of the DESC project, Journal of Loss Prevention in the Process Industries 20, 291–302.

Skjold T., Van Wingerden K., Hansen O.R., Eckhoff R.K., 2008, Institution of Chemical Engineers Symposium Series 154, 838-850.

Tezok F.I., Kauffman C.W., Sichel M., Nichols J.A., 1986, Turbulent burning velocity measurements for dust air mixtures in a constant volume spherical bomb, Progress in Astronautics and Aeronautics 105, 184–195.

Worsfold S. M., Amyotte P.R., Khan F.I., Dastidar A. G., Eckhoff, R. K., 2012, Review of the Explosibility of Nontraditional Dusts, Industrial & Engineering Chemistry Research 51 (22), 7651−7655.