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The Effect Of Turbulence On The Theoretical Evaluation Of Dust Explosions Severity

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The knowledge of thermo-kinetic parameters such as the maximum overpressure attained during an explosion (P_{max}) and the deflagration index (K_{St}) is starting point for sizing the equipment protection systems from dust explosions.
The experimental measurements of $K_{St.}$ and P_{max} are strongly dependent on the operating conditions and the chemico-physical characteristics of dust. The theoretical evaluation of such parameters is complicated by the fact that dust explosion proceeds through particle heating, heterogeneous combustion, devolatilization and homogeneous combustion; all of them strongly influenced by dust particle diameter.
In our previous paper (Di Benedetto & Russo, 2006) we calculated dust explosion thermo-kinetic parameters (K_{St}, P_{max}) by assuming that the pyrolysis/devolatilization step is very fast with respect to the other steps. We used a detailed reaction mechanism for the combustion of the volatiles. Preliminary results obtained at laminar conditions without taking into account the effect of turbulence were encouraging.
However, the deflagration index is strongly dependent on the turbulence level which is present in the experiments because it is needed for dispersing the dust and is generated when the cloud burns. In this work we extended our model to include the effect of the initial level of turbulence on the K_{St} values. We found that the effect of turbulence on K_{st} is almost negligible in standard test conditions, while it is significant at high initial turbulence level.

1 Introduction

The severity of dust explosions is usually expressed in terms of thermo-kinetic parameters such as the maximum overpressure attained during an explosion (P_{max}) and the deflagration index (K_{St}) which is a measure of the severity of the explosion.
The knowledge of these parameters is needed for sizing the equipment protection systems from dust explosions as they are used in the guidelines to protect and mitigate equipments from dust explosions. The evaluation of these parameters either experimental or theoretical is then required.
$K_{St.}$ and P_{max} are generally evaluated by means of explosion tests performed in properly designed vessels (1 m^3 vessel, 20 liter sphere) in which dusts are ignited at a proper time after their injection and dispersion. These measurements are strongly dependent on the operating conditions (i.e. dust dispersion degree, initial turbulence level) and the dust chemico-physical characteristics (i.e. particle size distribution and moisture content), (Cashdollar, 1996). As a consequence, the experimental evaluation of these parameters requires a strict control of turbulence level and dispersion degree.
Alternatively, modeling allows to give controlled values of such parameters by changing the simulation conditions. It is widely accepted that dust explosion occurs through heating, heterogeneous combustion, devolatilization and homogeneous combustion; which are all strongly influenced by dust properties (i.e. particle mean

diameter, size distribution). As discussed by Eckhoff (2003) many models have been proposed in the literature which simulate all or some of these steps by adopting a one-step reaction rate to describe both the heterogeneous and the homogeneous paths. At diameters lower than a critical value dust explosion is mainly controlled by homogeneous combustion: dust explosion is controlled by combustion of volatiles (Cashdollar et al., 1988, Yoshizawa & Kubota, 1982).
Accordingly, in our previous paper (Di Benedetto & Russo, 2006) we calculated dust explosion thermo-kinetic parameters (K_{St}, P_{max}) by assuming that the dust explosion is controlled by the volatiles combustion step. By using a detailed reaction mechanism, we calculated $K_{St,}$ S_l, P_{max} for corn starch, cellulose and polyethylene and we obtained a good agreement with the experimental values. Such results were obtained by assuming laminar flow conditions. The model results were compared with the data of K_{st} available in the guidelines (NFPA68, 2002)obtained at standard conditions. The agreement was very good since in the test case conditions the turbulence level is quite low and then no significant differences between the laminar and turbulent conditions apply.
In conditions different from the standard test case, strong turbulent flow may be present then significant deviation from the laminar case may exist (Lee et al., 1987; Amyotte et al., 1988; Pu et al., 1990; Tamanini & Ural, 1992; van der Wel et al., 1992; Eckhoff, 1992; Gieras et al., 1995; Dahoe et al., 2001).
In the present work we then extended our model to take into account the effect of the initial turbulence level on the K_{St} values.

2. Model

We calculated the deflagration index (K_{St}) by using the formula of Lewis von Elbe here reported:

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

where the maximum pressure rise (dP/dt_{max}) is calculated according to the formula recently proposed by Dahoe et al. (1996):

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

where: P_{max} is the maximum pressure reached in a closed vessel which has been calculated by using the equilibrium module of the CHEMKIN code; P_o is the initial pressure (1 bar); R_{vessel} is the radius of the reference spherical vessel ($1m^3$) and S_u is the burning velocity.
To take into account the effect of turbulence, S_u is assumed equal to turbulent burning velocity (S_t). S_t was calculated as function of the turbulence level (u^I) and of the laminar burning velocity by means of different formulas (Table I). As previously described (Di Benedetto & Russo, 2006), the laminar burning velocity was calculated as that relevant to the volatiles produced from the dust pyrolysis/devolatilization step. In particular, the calculation of S_l was carried out by means of simulations of the one-dimensional, planar, adiabatic, steady, unstretched, laminar flame propagation. The Sandia PREMIX module of the CHEMKIN package was used by implementing the detailed reaction scheme GRI-Mech 3.0 (Bowman et al., 1999). The gas composition of volatiles was obtained from literature data. In particular, we found the best agreement between simulation and experimental results for corn starch by using the volatiles composition data of Encinar et al. (1997).

3. Results

In dust explosion tests, dust clouds are usually formed by means of a pneumatic dust dispersion system. During dust dispersion, intensive turbulence will be inevitably induced in dust air mixtures, but it has the feature of decaying in its intensity with time. A dust cloud can be ignited by a defined delay time from beginning of dust dispersion and, hence at a given initial level of turbulence.

In order to evaluate the deflagration index as function of the turbulence level (eq.2) the turbulent burning velocity as function of turbulence has to be known. But in both gas and dust explosions the evaluation of the turbulent burning velocity as function of the turbulence intensity is hard task.

Furthermore, several combustion regimes may be experienced as function of the local conditions and a single model is not able to describe the burning velocity in all the combustion regimes. From the regime diagram for turbulent premixed combustion, it is found that in the range u^I/S_l of interest for the present model (≤ 20), the regime is flamelets. Depending on the ratio between the vessel length and the flame thickness the passage from wrinkled to corrugated and/or to thin reaction zones regime may occur. In a vessel volume (1 m^3 or 20 l) with a flame thickness of 10 mm, we may expect that the regimes which establish are always the wrinkled and the corrugated regimes. In the wrinkled and corrugated combustion regime, a large-scale turbulence establishes in which the interaction between a flame front and the turbulent flow field is purely kinematic. In this regime, according to Damköhler, the increase of the burning velocity is due to the increase of the flame area which is proportional to the increase of flow velocity over the laminar burning velocity, according to the following relationship:

$$\frac{S_t}{S_l} = 1 + \frac{u^I}{S_l} \tag{3}$$

where the velocity increase has been identified as the r.m.s velocity (u^I).

Pocheau (1994) generalized this model showing that also in the corrugated flamelets regimes the following formula is valid which satisfies the scale invariance:

$$\frac{S_t}{S_l} = \left[1 + \beta\left(\frac{u^I}{S_l}\right)^n\right]^{1/n} \tag{4}$$

where β may varies between 1-20 and n is generally assumed as equal to 2.

In the years many attempts have been performed to correlate the experimental data of turbulent burning velocity of both gases and dusts, by using expression (3) in a more generalised form:

$$\frac{S_t}{S_l} = 1 + A\left(\frac{u^I}{S_l}\right)^b \tag{5}$$

where A and b are empirical parameters.

Phylaktou et al. (1992) performed a fitting of 769 experimental data from 25 publications of S_T as function of u^I by using equation 5, in which u^I/S_l varies from 0 to 100. They found the values of constants A = 2, b = 1, which are also in agreement with theoretical models.

In Table 1 some formulas available from literature for the turbulent burning velocity as function of the turbulence level are reported : formula 1-4 were obtained for dusts, while formula 5-7 were obtained for gases.

Concerning dust explosions, a similar approach has been followed. One of the first work comes from Tezok et al. (1986), where experiments on maize starch mixtures at two

concentrations (300, 750 g/m^3) were performed in a 0.95 m^3 spherical bomb. Tezok et al. (1986) found a single relationship for two maize starch mixtures: the turbulent burning velocity normalised by the laminar burning velocity increased linearly with the turbulence intensity normalised by the laminar burning velocity (formula *1*, Table 1).
Gieras et al. (1995) developed a combustion model on the basis of experiments in a 1.25 m^3 spherical explosion bomb. The experiments allowed for estimating burning velocity as function of the turbulence intensity for different dusts: lycopodium, wheat and maize starch. The model gives a linear increase of the turbulent burning velocity with turbulence intensity (formula *2*, Table 1) through a dust dependent coefficient (K): K = 0.37 for lycopodium, K = 0.16 for wheat and K = 0.46 for maize starch.
Zhen & Leuckel (1996) investigated the influence of u^I on the turbulent burning velocity of corn starch air mixtures in a 1 m^3 cylindrical vessel and found a linear relationship between the turbulent burning velocity and the square root of the turbulent intensity (formula *3*, Table 1).

Table 1 – Formulas of turbulent burning velocity

Number	S_t (m/s)	Dust/Gas	Reference
1	$S_l + 0.45u'$	Dust	*Tezok et al.,1986*
2	$S_l + Ku'$	Dust	*Gieras et al. 1995*
3	$S_l \cdot \left(1 + 1.65 \cdot \frac{u'^{0.5}}{S_l}\right)$	Dust	*Zhen & Leuckel, 1996*
4	$6.8 \cdot S_l^{0.6} l_t^{0.15} u'^{0.15}$	Dust	*van Wingerden et al., 2001*
5	$S_l \cdot \left(1 + 2 \cdot \frac{u'}{S_l}\right)$	Gas	*Phylakotu et al., 1992*
6	$S_l \cdot \left(1 + \left(\frac{u'}{S_l}\right)^2\right)^{0.5}$	Gas	*Pocheau, 1994*
7	$S_l \cdot \left(1 + \left(\frac{u'}{S_l}\right)^2\right)$	Gas	*Gulder, 1990*

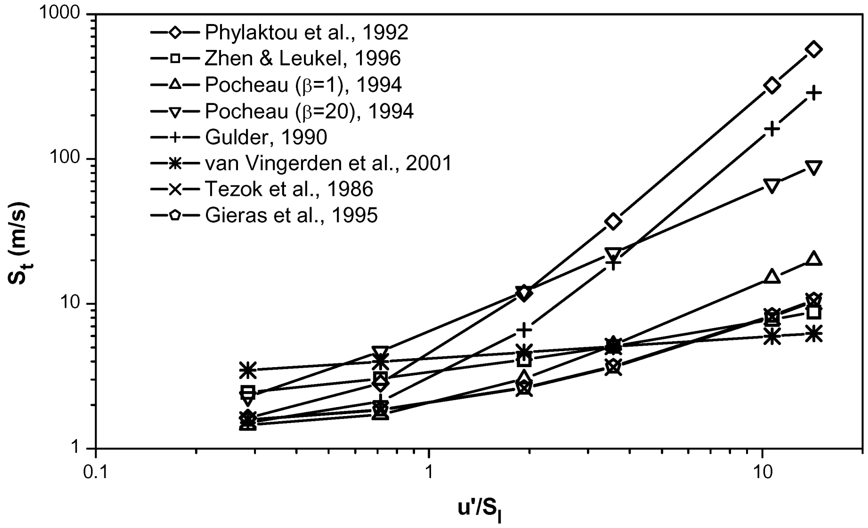

Figure 1 – Turbulent burning velocity (S_t) as function of u^I/S_l for corn starch at stoichiometric concentration (C=230 g/m^3, S_l = 1.4 m/s).

In Figure 1, the values of S_t for corn-starch calculated at the stoichiometric concentration (C = 230 g/m^3; S_l = 1.4 m/s) by using all the formulas in Table 1 are reported as function of the u^I/S_l ratio.

At low value of the u^I/S_l ratio, all the formulas give almost the same S_t value except those of van Wingerden et al. (2001), Zhen & Leukel (1996) and Pocheau (1994) (β=20) which give higher values. Increasing the u^I/S_l ratio (>1), the S_t given by formula *5* (Phylakotu et al., 1992) and *7* (*Gulder, 1990)* increases more than that obtained by other formulas.

We then calculated the deflagration index (K_{St}) as function of the turbulence level (u^I) using equation (2) replacing S_u with the S_t here calculated and reported in Figure 1.

In Figure 2 the K_{St} profiles for corn-starch at stoichiometric concentration are reported as function of u^I/S_l ratio. The model results show that the deflagration index calculation is strongly sensitive to the turbulent burning velocity. In the standard conditions of test vessels for experimental evaluation of K_{St} (NFPA68, 2002), the turbulence level is about u^I = 0.4 m/s. At this value, the effect of turbulence on the S_t and then on K_{st} is almost negligible and all the values collapse, except those coming form van Wingerden et al. (2001), Zhen & Leuckel (1996) and Pocheau (1994) (β=20). Conversely, at higher level of turbulence (u^I > 1 m/s) which can be easily encountered in industrial plants, the deflagration index is significantly affected by the turbulence level and then the correct prediction of S_t is required to evaluate the violence of explosion (K_{st}) and then to classify the dust hazard.

According to the results shown in Figure 2 it appears that the K_{St} value increase 10 times when u^I increase about 10 times, as also found in previous experiments (Lee et al., 1987; Amyotte et al., 1989; Pu et al., 1990; Tamanini & Ural, 1992; Gieras et al., 1995; Dahoe et al., 2001).

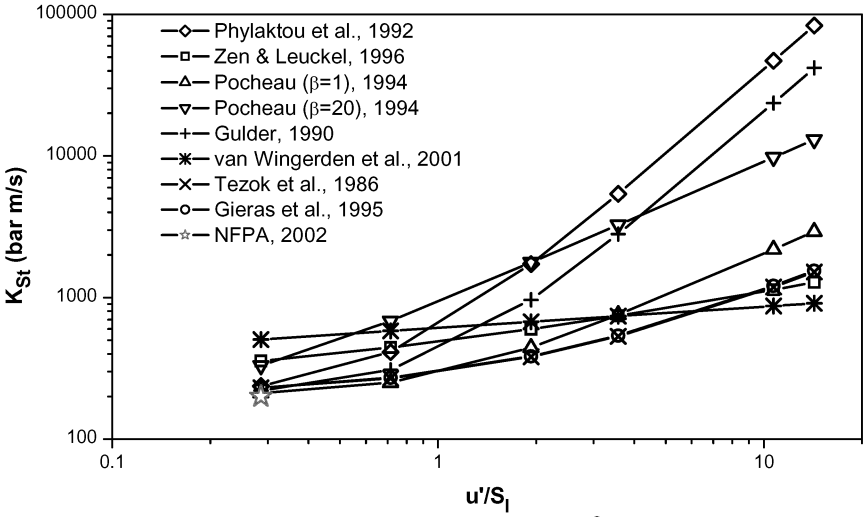

Figure 2 – Deflagration index (K_{st}) as function of u^l/S_l for corn starch at stoichiometric concentration ($C=230$ g/m^3).

4. Conclusions

The here developed model allows the calculation of the maximum pressure and the deflagration index once the composition of pyrolysis gas products and the initial level of turbulence is known. In particular, the effect of the initial turbulence on K_{St} is more pronounced at $u^l > 1$ m/s which can be easily encountered in industrial plants, and then the correct prediction of S_t is required to evaluate the violence of explosion (K_{st}) and eventually to classify the dust hazard.

5. References

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