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# A kinetic free mathematical model for the prediction of the $K_{St}$ reduction with the particle size increase



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### ABSTRACT

Even in recent years, several major industrial accidents have involved dust explosions, clearly showing the necessity of mitigating the hazard related to the presence of flammable dusts. In this respect, the  $K_{st}$  is an experimental parameter used to design the deflagration vents aimed to protect industrial devices and silos by internal dust explosions. Even if it is measured using a standard 20 L sphere test, its determination is quite expensive and time consuming. This problem is even more severe when a target dust is processed into a plant, giving rise to different average diameters; in this case, an experimental investigation of all the different particle sizes would be advisable but very expensive. In this context, the main aim of the present paper has been to develop a kinetic-free model able to predict the K<sub>St</sub> decrease with the mean particle diameter increase for organic dusts explosions. Particularly, an order of magnitude analysis of the characteristic times of the involved phenomena has showed that, in the  $K_{St}$  measurements, the rate determining step is usually associated to heat transfer phenomena. This evidence leads to the possibility of exploring a predictive approach for the  $K_{St}$  determination which does not require any chemical kinetic information, the most difficult to be obtained. Therefore, once the value of  $K_{St}$  has been measured through a standard 20 L test for a given mean particle diameter (the smallest possible), the approach proposed in this work allows for predicting the  $K_{\rm sr}$  values for the same dust at higher average particle sizes. Such an approach has been validated by comparison with several literature data as well as with a new set of experimental results.

### 1. Introduction

It is well known that, in the last 50 years, a significant number of accidents have plagued the process industry. The classification of the consequences and causes of such accidents has permitted to identify five main classes of involved phenomena (often more than one of them is usually involved in a single accident): fires (CBS, 2018; ARIA, 2018; Wehmeier and Mitropetros, 2016), runaway reactions (CBS, 2018; ARIA, 2018; Pasquet, 2017; Casson Moreno et al., 2016, 2014; Copelli et al., 2010, 2011, 2014), gas and dust explosions (CBS, 2018; ARIA, 2018; Bershad, 2017; Eckhoff, 2003), toxic releases (CBS, 2018; ARIA, 2018) and hazardous spilling of liquids (CBS, 2018; ARIA, 2018). Particularly, in recent years, several major industrial accidents have involved dust explosions; most of them also affected industrial plants where the same organic dust was present in separated areas with different mean diameters. For the sake of example: the 2003 polyethylene dust explosion in North Carolina, USA; the 2008 sugar powder explosion in Georgia, USA; the 2015 flour mill explosion (where 4 workers

### were killed) in United Kingdom (CBS, 2018; DUST\_EXPLOSION\_RESEARCH, 2018).

This is relevant because the violence of a dust explosion (usually summarized in the value of an experimental parameter, the deflagration index  $K_{St}$ ), is strongly affected by the particle size distribution (quite often represented in an effective way by the mean particle diameter) of the analyzed organic dust (Eckhoff, 2003). In particular, it is well established that the deflagration index (and, consequently the explosion hazard related to a given dust) decreases when the mean dust diameter increases (Eckhoff, 2003; Abbasi and Abbasi, 2007; Di Benedetto et al., 2010; Mittal, 2015).

The deflagration index is an experimental parameter used to characterize the violence of the explosion of a given dust cloud and, consequently, it is the main parameter used to design the deflagration vents aimed to protect industrial devices and silos by internal dust explosions (NFPA, 2013). It is usually measured using a standard 20 L apparatus test (Siwek, 1977), which is easier to use than the 1 m<sup>3</sup> sphere that requires a larger amount of dust and more time for cleaning operations,

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even if some limitations related to the use of the standard 20 L apparatus have been reported in the literature (underlined in a recent review by Fumagalli et al., 2016). Apart from these limitations, the measure of the  $K_{St}$  value through this apparatus requires quite a large number of tests, and therefore a quite large amount of dust. This is not a trivial problem when very expensive dusts are involved, as usual for instance in the pharma industry.

Hence, in the last years, some different mathematical models have been proposed to predict the K<sub>st</sub> value for a given organic dust (Callé et al., 2005; Di Benedetto et al., 2010; Russo et al., 2013; Mittal, 2015). However, all the proposed approaches basically represent the phenomena involved in the standard 20 L sphere test with a two-regions model: the first region is that of the unburnt particles, while the second one is that of the burnt particles; the two regions being separated by the flame region that propagates towards the unburnt particles. Therefore, the explosion proceeds thanks to the heating of the unburnt particles by the flame, which leads to the release of flammable gases, which sustain the flame propagation. Consequently, these approaches share the necessity to represent correctly the kinetics of the chemical reactions involved, from the initial pyrolysis of the organic matter up to the combustion reactions of the flammable gases released from the heated particles. This is an important bottleneck as such kinetic information are usually unavailable, and a detailed kinetic characterization of the dust combustion can require much more resources than performing the standard 20 L test.

Therefore, the main aim of the present paper is to develop a kineticfree model (both pyrolysis and combustion) able to predict the  $K_{St}$  change with the mean particle size for organic dusts explosions. In other words, once the value of the deflagration index has been measured through the standard 20 L test for a given average particle diameter, the proposed approach allows for predicting the  $K_{St}$  values at different dimensions of the same dust without knowing any chemical kinetic information. This imply the possibility to save a significant amount of resources when the same dust is present in separated working areas with different mean diameters. Moreover, the proposed approach has been validated by comparison with four sets of literature data as well as with a new set of experimental results.

#### 2. Experimental dependence of $K_{St}$ on the mean particle diameter

As previously mentioned, it is well known that the experimental  $K_{St}$ value decreases with the mean particle diameter increase (Abbasi and Abbasi, 2007; Eckhoff, 2003). However, only a few of the experimental data available in the literature have been obtained under clearly detailed operation conditions (humidity, ignition delay time, nozzle type, cooling mode, state of cleanliness of the sphere wall), making them useful for understanding properly the relationship between  $K_{St}$  and particle diameter. In particular, in order to validate the approach discussed in the following section some literature experimental data have been used: polyethylene (Di Benedetto et al., 2010); sugar (GESTIS-Database, 2017); cornstarch (Mittal, 2015); and, niacin (Fumagalli et al., 2017), whose K<sub>St</sub> vs. particle diameter are summarized in Fig. 1. Moreover, the same figure also reports some new experimental data for wheat flour measured following the ASTM-E1226 standard (ASTM, 2012). Analyzing such data, it is possible to observe that the  $K_{St}$  values always decrease as the dusts mean diameters increase.

### 3. A new phenomenological model

In the standard 20 L sphere the ignition source in the measurements of the  $K_{St}$  value of a dust cloud is provided by two chemical ignitors, which are composed by a mixture of three different powders: 40% of zirconium, 30% of barium nitrate, and 30% of barium peroxide (ASTM, 2012). This is a multipoint ignition source (Zhen and Leuckel, 1997), where a spark generated between two electrodes located inside the capsules of the chemical ignitors causes the decomposition of both



Fig. 1. Experimental  $K_{St}$  values vs. mean dust diameter used to validate the proposed approach.

barium nitrate and peroxide, therefore leading to a sudden oxygen generation, which starts the fast and exothermic oxidation of the zirconium powder. Hence, after the capsule breaking due to the gas generation, a cloud of incandescent zirconium particles is dispersed within the sphere, leading to the ignition of the combustible dust. The energy released by the ignitors is equal to about 10 kJ, which creates a "fireball" quickly occupying the whole sphere volume. In other words, in a very short time, the dust cloud initially dispersed in the sphere at room temperature was wrapped in a mixture of hot gases and incandescent metal dusts.

The basic idea, which differences the proposed approach with respect to the others previous presented in the literature, is that the "fireball" created by the bursting of the ignitors at the beginning of the standard 20 L test is assumed to be instantaneous, therefore creating a hot environment in which all the particles are suddenly embedded. This assumption is supported by the experimental evidence shown in Fig. 2 (which refers to the bursting of the ignitors in a sphere filled only with air, that is, without any flammable dust): it can be noticed that the pressure suddenly increases, due to the "fireball" propagation, in a few milliseconds after the ignitors' lighting.

Following this representation of the standard 20 L test, it is



Fig. 2. Experimental pressure increase into the 20 L sphere filled with air.

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