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Effects of the mean particle size on the deflagration index estimation for cornstarch dust

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Abstract

The National Fire Protection Association (NFPA) defines the dust explosions as a "credible risk". Hence, to meet the challenge to prevent and protect from the catastrophic effects of these phenomena, it is fundamental to know what are the characteristics and the burning conditions regarding the combustible dusts that could have an effect on the explosion violence. The K_{St} , also known as deflagration index, is one of the relevant parameters in dust explosions, together with the maximum explosion overpressure generated in the test chamber, the minimum ignition energy and so on. In particular, the deflagration index measures the relative explosion severity and it is used in the design of the dust venting protection equipment. However, one of the criticalities of such a parameter is that is strongly affected by the particle mean diameter. Hence, in the following, it will be preliminary presented the validation of a single particle spherical model able to predict the variation of the deflagration index with the increasing mean particle size knowing just one experimental K_{St} value.

Introduction

Dust explosions could be catastrophic considering both workers' safety and industry damages. For this reason, in the last years, the dust explosion phenomenon has been extensively investigated. For the sake of example, the U.S Chemistry Safety Board [1] strongly underlines hazards and risks related to combustible dusts, by studying accidents such as the one occurred at "Imperial Sugar Company", where 14 people were killed, 40-50 were injured and the entire plant was devastated. To prevent and protect from the consequences of this phenomenon, knowing the expected violence generated by the dust explosions is crucial. The parameter, which better summarizes this information, is the deflagration index; however, for dusts, the K_{St} is strongly dependent upon the mean particle diameter. This could be interesting in all the industries where granulating and milling process are conducted in separated areas of the same plant. In this case, a complete characterization of the hazard related to the dust should require a large amount of resources conducting several test in standardized equipment [2]. For this reason, recently certain mathematical models able to predict the deflagration index values

have been proposed [3]. The possibility to have reliable mathematical model should allow strongly reducing the resources required in the hazard assessment procedure, especially for SMEs. In this study the validation of a single particle model able to predict the effects of the mean particle size on the deflagration index value has been performed with reference to literature data available for maize starch [4].

Mathematical Model

The organic dusts, such as maize starch, mainly burn through a homogeneous mechanism; so the gas-phase combustion follows the pyrolysis/devolatilization process [5]. In the last decade, different single particle models able to predict the variation of the K_{St} as a function of the particle mean diameter have been presented [6-7]. These approaches are based on the following assumptions: 1) pyrolysis kinetic model is used to evaluate the volatiles production rate and 2) the K_{St} at different diameters is evaluated as a function of the volatiles production rate. Along the same lines, in the present study a spherical single particle model has been developed. The model is able to extrapolate the deflagration index value for a given dust diameter respect to an experimental value of the K_{St} at a reference diameter and it was developed under the subsequent hypotheses:

- 1) a flame front is generated in the 20 L sphere by the instantaneous combustion of volatiles previously released by other burning particles;
- 2) the equations are written in spherical coordinates;
- 3) negligible resistance to mass transfer and negligible diffusive flux;
- 4) pyrolysis products are not involved in secondary reactions, apart from the combustion reaction;
- 5) local thermal equilibrium between solid and volatiles;
- 6) pseudo steady-state conditions for the gas phase;
- 7) a solid skeleton is generated by the carbon residue, so the particles volume can be considered as constant;
- 8) the mass and molar specific velocities are equal;
- 9) variations of the apparent solid density, in the energy balance equation, are taken into account by a mean effective solid density, assumed constant.

Pyrolysis/devolatilization process has been described following a single step global reaction from the solid particle (S) to the volatile phase (V). The resulting equation system derived from the aforementioned hypotheses is as follows:

$$\frac{\partial \bar{\rho}_S}{\partial t} = -r \quad (1)$$

$$\frac{\partial(\varepsilon \cdot \rho_G)}{\partial t} = r - \frac{\partial v}{\partial r} - \frac{2 \cdot v}{r} \approx 0 \quad (2)$$

$$\rho_{S,eff} c_{p,S} \frac{\partial T}{\partial t} = \bar{\lambda} \frac{\partial^2 T}{\partial r^2} + \frac{2 \cdot \bar{\lambda}}{r} \frac{\partial T}{\partial r} - c_{p,V} \left(\frac{\partial(v \cdot T)}{\partial r} + \frac{2 \cdot v \cdot T}{r} \right) - \Delta H_{rxn} r \quad (3)$$

In the solid mass balance equation, $\bar{\rho}_s$ is the ratio between the dust particle reacting mass and initial volume, V_0 , and r is the single-step reaction rate equal to $k \cdot \bar{\rho}_s^n$ where k has been evaluated according to the procedure described by Fumagalli et al. [7]. The kinetic parameters, evaluated for maize starch, are summarized in Table 1.

Table 1. Kinetic parameters estimated from TG measurements for maize starch

Parameter	Unit of measure	Value
Pre-exponential factor (A)	m^6/kg^2	$1.168 \cdot 10^{10}$
Activation Energy (E_{att})	J/mol	$1.775 \cdot 10^5$
Reaction Order (n)	-	3.0
Conversion factor (x)	-	0.188

In the Equation (2), v is the flux of volatiles that leaves the particle surface equal to $U_r \cdot \varepsilon \cdot \rho_G$, where U_r is the outward volatiles velocity, ρ_G is the ratio of the mass of volatiles with respect to the particle volume and ε is the particle porosity.

In the energy balance equation, $\rho_{s,eff}$ is the effective solid density equal to $\rho_{s,0} \cdot (1 - \bar{\varepsilon})$, where $\bar{\varepsilon}$ is a mean porosity, considered equal to 0.5, $\bar{\lambda} = \lambda \cdot (1 - \bar{\varepsilon})$ is the thermal conductivity referred to the solid phase; $c_{p,s}$ and $c_{p,v}$ are, respectively, the specific heat of solid and volatiles and ΔH_{rxn} is the pyrolysis reaction enthalpy. The system can be solved specifying both initial, Equations (4), (5a) and (5b), and boundary conditions:

$$\begin{cases} \bar{\rho}_s = \rho_{s,0} \cdot (1 - \beta) \\ T = T_0 \end{cases} \quad (4)$$

where β is the mass fraction that is not consumed by the pyrolysis/devolatilization process [7];

$$\begin{aligned} r = 0 &\rightarrow v = 0 \\ r = 0 &\rightarrow \frac{\lambda}{\rho_{s,0} \cdot c_{p,s}} \frac{\partial T}{\partial r} = 0 \end{aligned} \quad (5a)$$

$$r = R \rightarrow \frac{\lambda}{\rho_{s,0} \cdot c_{p,s}} \frac{\partial T}{\partial r} = -\frac{h_c \cdot (T - T_{ext})}{\rho_{s,0} \cdot c_{p,s} \cdot (1 - \bar{\varepsilon})} - \frac{e \cdot \sigma \cdot (T^4 - T_{ext}^4)}{\rho_{s,0} \cdot c_{p,s} \cdot (1 - \bar{\varepsilon})} \quad (5b)$$

where R is the particle radius, e is the emissivity, σ is the Stefan–Boltzmann constant and T_0 is the initial particle temperature, considered equal to 300 K. The external flame temperature, T_{ext} , is considered equal to the adiabatic flame temperature of methane, which is the major pyrolysis product that contributes to the combustion reaction (pyrolysis data have been taken from literature [4]). The

heat transfer coefficient, h_c , has been computed as reported in Çengel [8]. To predict the K_{St} value for a specific dust mean diameter, it has been used a formulation similar to the one proposed by Di Benedetto et al. [6]:

$$K_{St}(d) = \frac{VPR(d)}{VPR(d_1)} \cdot K_{St}(d_1) \quad (6)$$

where $VPR(d) = \max(v(r=R, t))$ is the maximum production rates of the volatile leaving the particle at the desired diameter (d) and at the reference one (d_1) and $K_{St}(d_1)$ is the reference experimental value of K_{St} measured in the 20 L sphere. The values of the maximum production rates were evaluated by solving the partial derivative-algebraic equation system (1-3) for all the different diameters, which needs to be investigated.

Results and discussion

For the calculations a reference diameter of about 22 μm was chosen for maize starch particles, with a K_{St} of about 162 bar m s^{-1} [4]. The parameters needed to evaluate the maximum volatiles production rate are reported in Table 2.

Table 2. Model parameters referred to maize starch

Parameter	Value	Parameter	Value
$\rho_{S,0}$	1480 kg/m^3 [4]	e	0.95 [10]
C_p	1880 J/(kg K) [4]	β	0.11
λ	0.216 W/(m K) [4]	T_{ext}	2226 K [11]
C_v	2125 J/(kg K) [9]	ΔH_{rxn}	8×10^5 J/kg [12]

The volatile heat capacities and the flame temperature for maize starch are also referred to methane such as the external gas temperature. The emissivity and pyrolysis enthalpy are supposed of the same order of magnitude and comparable to a disaccharide. A typical comparison of the particle heating history computed by the mathematical model, previously described, is shown in Figure 1.

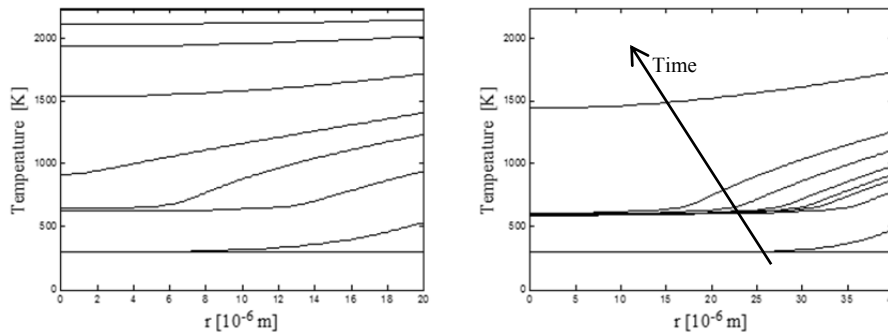


Figure 1. Heating history of particles with different sizes: 20 μm (left-side) and 40 μm (right-side).

As it is possible to see, considering the same reference time, the particles are affected by the external heating in different ways: the smaller particle reaches the external temperature in about 20 ms, the other one needs about 60 ms to reach the same temperature level. Hence, the bigger the dust particle is, the slower the heating and consequently the pyrolysis phenomena are, therefore resulting in a milder dust explosion. This is confirmed by Figure 2, where the volatile production rate as a function of time is plotted; as expected the trends present a maximum value, which decrease with the particle size increase. Therefore, the predictions of K_{St} as a function of the mean particle diameter are summarized in Figure 3; a good agreement with the experimental data of maize starch is highlighted.

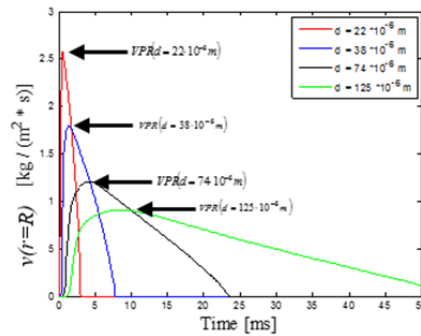


Figure 2. $v(r=R)$ vs. time trends for different particle diameters

The main assumption of this model is that the combustion reaction follows the pyrolysis/devolatilization process; to validate this hypothesis, predictions have been made with two different relative turbulent gas velocity, as reported in the plots of Figure 3, considering the velocity fluctuation equal to 2.68 m s^{-1} , typical value of the 20 L sphere after 60 ms from the injection [13]:

- 1) laminar velocity of the dust [14], coupled with the turbulent velocity evaluation according to Tezok et al (1986) [15], left part of Figure 3;
- 2) laminar velocity of methane [11], coupled with the turbulent velocity evaluation according to Pocheau (1994) [16], right part of Figure 3.

As it is possible to see, the curves are almost the same in the two cases analysed. Hence, it is possible to say that the assumption on the external combustion driven only by the volatiles phase is worthy, underlining once again that for organic dusts the homogeneous mechanism is dominant with respect to the heterogeneous one. In this case, the experimental determination of the dust burning velocity can be substituted with a similar information about the volatiles pyrolysis.

Conclusions

In this paper, it has been proposed and validated a spherical particle model able to predict the effects of the mean particle size on the K_{St} index.

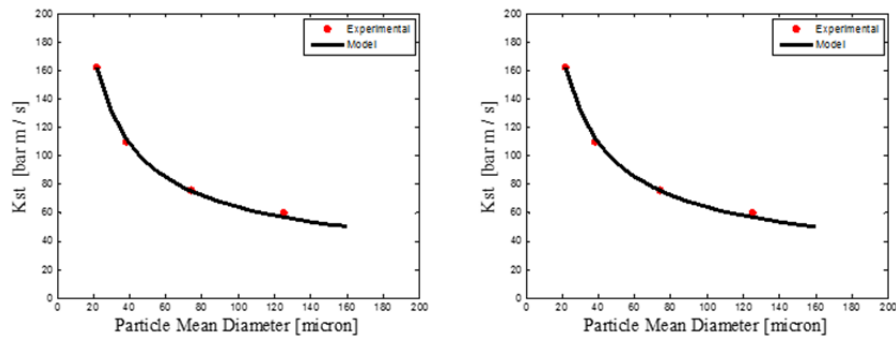


Figure 3. Results obtained for different laminar velocities: dust (left), CH₄ (right).

In addition, it has been shown that, for organic dusts, considering just the gas/vapour combustion is a realistic assumption; this could substitute the knowledge of the complex burning mechanism that takes place during the dust explosions even if this method is still dependent from an experimental measurement.

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