

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_{St} 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_{St} 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.

Keywords: Organic Dust Explosion; Deflagration Index; Explosion Severity; Modeling; Experimental data; Kinetic-free Model.

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; Bershada, 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 m³ sphere that requires a larger amount of dust and more time for cleaning operations, 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_{St} 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 kinetic-free 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 implies 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 the 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 the 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_{St} vs. particle diameter are summarized in Figure 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 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 differentiates 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 Figure 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 interesting to evaluate which phenomenon controls the explosion violence; that is, the measured K_{St} value. As far as organic dusts are involved, it is well known that the particle combustion usually proceeds through a series of steps (Fumagalli et al., 2016), namely: the heat is transferred from the environment to the particle surface (external heating step); the heat is transferred from the particle surface inward (internal heating step); the heated particle decomposes generating some flammable gases (pyrolysis/decomposition step); the flammable volatiles exit the particle and burn with the surrounding air (combustion step). To each of these steps can be associated a characteristic time value, which is representative of the step velocity; if a step shows a characteristic time much larger than the other steps it controls the overall particle explosion rate and, as a consequence, the violence of the explosion.

The characteristic time of the external heating step (t_e) can be estimated from the convective contribute to the heat transfer as:

$$t_e = \frac{c_{p,S} \cdot \rho_{S,0} \cdot d}{h_c} \quad (1)$$

where h_c is the external heat transfer coefficient between gas and solid particle evaluated through standard correlations developed for turbulent conditions, which are typical of a 20 L sphere experiments (Pu et al., 1990; Zhen and Leuckel, 1996; Dahoe et al., 2001; Dahoe et al., 2002); d is the characteristic particle

length, represented by the particle mean diameter; $\rho_{S,0}$ is the initial solid density; and, $c_{p,S}$ is the average specific heat of the solid.

The characteristic time of the internal heating step (t_i) can be estimated as:

$$t_i = \frac{c_{p,S} \cdot \rho_{S,0} \cdot d^2}{\lambda} \quad (2)$$

where λ is the particle thermal conductivity.

The characteristic time of the pyrolysis/decomposition step (t_r) can be estimated from the pyrolysis reaction rate equation as:

$$t_r = \frac{1}{k \cdot (\rho_{S,0} \cdot (1 - \beta))^{n-1}} \quad (3)$$

where k is the kinetic constant of the pyrolysis/devolatilization chemical reaction. As discussed elsewhere (Fumagalli et al., 2017), such a kinetic constant can be estimated by: 1) carrying out thermogravimetric (TG) tests on the dust to be analyzed; 2) writing a mass balance equation describing the material loss due to increasing temperature.

In order to consider only the reacting solid that contributes to the pyrolysis/devolatilization process, the solid mass (m_s) vs temperature (T) data of the TG experiment have been processed by subtracting a quantity equal to $m_{S,0} \cdot \beta$, being $m_{S,0}$ the initial mass and β the ratio between the mass of the final residue ($m_{S,end}$) and $m_{S,0}$. This process generates a new mass variable defined as $\overline{m}_s(T) = m_s(T) - m_{S,0} \cdot \beta$, with an initial value equal to $\overline{m}_{S,0} = m_{S,0} \cdot (1 - \beta)$ and a final value equal to $\overline{m}_{S,end} = m_{S,0} \cdot \beta - m_{S,0} \cdot \beta = 0$. By definition, the final conversion of the reacting solid (α) is always complete and it is defined as:

$$\alpha = \frac{\overline{m}_{S,0} - \overline{m}_s}{\overline{m}_{S,0}} = \frac{m_{S,0} \cdot (1 - \beta) - (m_s - m_{S,0} \cdot \beta)}{m_{S,0} \cdot (1 - \beta)} = \frac{m_{S,0} - m_s}{m_{S,0} \cdot (1 - \beta)} \quad (4)$$

For the sake of example, the solid conversion measured in a TG experiment on wheat flour is shown in Figure 3. These data can be used to estimate the kinetic parameters of a one-step pyrolysis reaction leading

to volatiles (V) from a reacting solid (S):



The mass balance equation on the mass used in the TG analysis (in terms of reacting solid conversion) can be written as (Fumagalli et al., 2017):

$$\frac{d\alpha}{dt} = A \cdot e^{\left(\frac{E(1-x\alpha)}{R \cdot T}\right)} \cdot [\rho_{S,0}(1-\beta)]^{n-1} \cdot (1-\alpha)^n \quad (6)$$

where a modified Arrhenius expression has been used. In this relation R is the universal gas constant, T is the temperature, α is the gravimetric conversion of the reacting solid (evaluated from the mass loss), χ is a correction factor making the activation energy value (E) depending on the solid conversion and n is the reaction order. This dependence accounts in an effective way for the solid composition change during the pyrolysis process and allows for describing the pyrolysis kinetics using a simple lumped reaction.

The values of the estimated kinetic parameters are summarized in Table 1, while the fitting results on wheat flour are compared with the experimental ones in Figure 3 in terms of solid conversion vs. temperature. This will allow, using e.g. the kinetic data summarized in Table 1, for estimating the characteristic time of pyrolysis, as discussed above.

The characteristic time of the homogeneous combustion step (t_c) can be estimated as:

$$t_c = \frac{S}{\delta} \quad (7)$$

where δ is the flame thickness, normally of the order of 1 mm (Di Benedetto et al., 2010) and S is the turbulent burning velocity that can be estimated as (Zhen and Leuckel, 1997):

$$S = S_j \cdot \left(1 + 3.5 \cdot \frac{u'^{0.5}}{S_j}\right) \quad (8)$$

where S_j is the laminar burning velocity (Hattwig and Steen, 2004), and u' is the velocity fluctuation, which has been estimated to be, in the 20 L sphere after the usual delay time of 60 ms (ASTM, 2012), equal to 2.68 m/s (Dahoe et al, 2001).

For the sake of example, Figures 4 summarize the estimated characteristic time values for respectively: wheat flour with a particle diameters of about 48 μm (Figure 4a) and 351 μm (Figure 4b), niacin with a particle diameter of 20 μm (Figure 4c) and sugar at 300 μm (Figure 4d). We can easily observe that, starting from about 500-600 K, the slowest phenomena are those related to the heat transfer, while those ones related to the chemical reactions (that is, pyrolysis and combustion) become much faster.

Reminding that the K_{St} value for a given dust is experimentally determined from the maximum value of the pressure rate in the standard 20 L sphere test, $K_{St} = (dP/dt)_{\max} \cdot 0.02^{1/3}$, and that, coherently with the assumed physical sketch of the phenomena, all the particles are suddenly embedded in a hot environment and burnt all together, the values of the characteristic times should be compared at the temperature value reached in the sphere when the pressure rate is maximum in order to identify, if it exists, the rate determining step (that is, the slowest step) for the K_{St} determination. Such a temperature value can be easily computed using the ideal gas law from the pressure value reached in the sphere when the pressure rate is maximum. For the sake of example, from the experiments carried out in the 20 L sphere with wheat flour, temperature values ranging from about 750 up to 1450 K (for average particle diameters from about 350 μm down to about 50 μm , respectively) have been computed, which are clearly beyond the threshold limit of 500-600 K evidenced by Figure 4a and Figure 4b. Similar conclusions can be drawn for the other dusts.

These evidences lead to assume that, at least as a first approximation, the changes in the explosion violence (that is, in the experimental K_{St} value) when changing the particle diameter of a given dust are mainly connected to the heat transfer phenomena rate, which can be represented, at a glance, by the initial heating rate of a particle caused by the “fireball” generated by the bursting of the ignitors. This assumption can be recast in the following relation:

$$K_{St}(d) = \frac{\frac{\partial T}{\partial t}(t=0, r=d/2)}{\frac{\partial T}{\partial t}(t=0, r=d_{ref}/2)} \cdot K_{St}(d_{ref}) \quad (9)$$

where d_{ref} is a reference average particle diameter, $K_{St}(d_{ref})$ is the experimental value of the deflagration index measured at that diameter, and $\partial T/\partial t(t=0, r=d_{ref}/2)$ is the derivative with respect to time of the temperature of the external boundary of a particle with diameter equal to d_{ref} . Analogously, $K_{St}(d)$ is the experimental value of the deflagration index predicted for an average diameter equal to d , and $\partial T/\partial t(t=0, r=d/2)$ is the derivative with respect to time of the temperature of the external boundary of a particle with diameter equal to d .

It should be stressed that this approach allows disregarding fully the chemical kinetic information since they are implicitly contained in the experimental value $K_{St}(d_{ref})$; in other words, once the value of the deflagration index is experimentally determined for a dust with an average particle diameter, equation (9) allows for predicting the value of K_{St} for the same dust with any other particle diameter value higher than the reference one, using only the estimation of the initial heating rate of the particle at its external boundary for both the diameters.

The initial heating rate of the boundary of a particle, disregarding any chemical reaction (since we are interested in the heating rate at the very beginning of the test), can be computed through a suitable mathematical model on the basis of the following assumptions:

- 1) the effective temperature of the gases surrounding the particle is reached almost instantaneously after ignitors' lighting and it can be roughly estimated from both the previously reported considerations about the characteristic times of the heat transfer and the pressure-time data reported in Figure 2: it is equal to about 500-600 K;
- 2) no chemical reactions;
- 3) the system is pseudo-one-dimensional in spherical coordinates;
- 4) spherical particles with constant volume;
- 5) the convective heat transfer coefficient between gas and solid particle (h_c) can be evaluated through standard correlations developed for turbulent conditions, which are typical of a 20 L sphere experiments (Pu

et al., 1990; Zhen and Leuckel, 1996; Dahoe et al., 2001; Dahoe et al., 2002).

From these assumptions, the energy balance equation for a particle becomes:

$$\rho_{S,0} \cdot c_{p,S} \cdot \frac{\partial T}{\partial t} = \lambda \cdot \frac{\partial^2 T}{\partial r^2} + 2 \cdot \frac{\lambda}{r} \cdot \frac{\partial T}{\partial r} \quad (10)$$

where r is the spherical coordinate. This equation has to be complemented with boundary and initial conditions as follows:

$$t, r = 0 \rightarrow \frac{\lambda}{\rho_{S,0} \cdot c_{p,S}} \cdot \frac{\partial T}{\partial r} \Big|_{r=0} = 0$$

$$t, r = R \rightarrow \frac{\lambda}{\rho_{S,0} \cdot c_{p,S}} \cdot \frac{\partial T}{\partial r} \Big|_{r=R} = -\frac{h_c}{\rho_{S,0} \cdot c_{p,S}} \cdot (T - T_{ext}) \quad (11)$$

$$t = 0, r \rightarrow T_{t=0} = T_0$$

where $R=d/2$ is the particle radius, T_{ext} is the effective temperature reached almost instantaneously after ignitors' lighting, and T_0 is the initial particle temperature (set equal to 300 K).

Equation (10) is a Partial Differential Equation that has been solved using the Method Of Lines (MOL) (Schiesser, 1991): spatial derivatives have been approximated through finite differences using 300 equidistant nodes and a five-point centred scheme (Vande Wouwer et al., 2014) has been implemented using a differentiation matrix evaluated with the Fornberg's procedure (Fornberg, 1998; Fornberg, 1988). This leads to a system of Ordinary Differential Equations (ODEs) whose numerical integration has been carried out through the MATLAB® ode15s function.

By integrating equation (10), the value of the initial heating rate of a particle with a given diameter to be used in Equation (9) can be easily estimated as previously indicated in Equation (9).

4. Validation and discussion

As discussed in several previous works (e.g., Eckhoff, 2003; Abbasi and Abbasi, 2007), the effect of increasing the particle size is to reduce the dust explosion violence as summarized in the K_{St} values reported

in Figure 1 for various average particle diameters and different dusts; the measured K_{St} .

For all these dusts, the smallest diameter value investigated experimentally has been selected as the reference value, d_{ref} . Moreover, the mathematical model previously discussed involves some other constitutive parameters, which are summarized in Table 2. Moreover, the heat transfer coefficient h_c has been computed as reported in Çengel (2008).

For all the dusts considered, the results obtained by integrating Equation (10) and then applying Equation (9) to predict the K_{St} values for average particle diameters different than the reference one are shown in the parity plot of Figure 5, where all the data but the ones used as a reference are summarized. We can see a fair agreement among experimental and predicted data for the investigated dusts. This is quite remarkable since the data reported in Figure 5 are true predictions, that is, no model parameters have been tuned on these experimental data. The largest errors have been found for a couple of low K_{St} values, where the model over predicts the experimental data. Such a conservative (from a safety point of view) behavior of the model should not be a major problem since it is confined to very low K_{St} values.

5. Conclusions

In this paper, a kinetic-free methodology to predict the K_{St} value of organic dusts as a function of their average particle diameter has been presented and validated by comparison with experimental values measured in the 20 L sphere for five different organic dusts: polyethylene, cornstarch, wheat flour, sugar and niacin.

The main novelties proposed in the paper are related to:

- 1) the description of the dust deflagration phenomena involved in the standard 20 L sphere test;
- 2) the order of magnitude analysis of the characteristic times of the phenomena involved.

Particularly, for what concerns the first point, instead of assuming the ignition of the dust cloud in a point from which a spherical flame front propagates, as usually done in the well known two-zone or three-zone models, the proposed approach assumes that the fireball created by the ignitors' lighting instantaneously

produces a hot environment in which all the particles are suddenly embedded.

Secondarily, the order of magnitude analysis of the characteristic times of the phenomena involved, showed that in the K_{St} measurement the rate determining step was usually associated to heat transfer phenomena.

These assumptions permit to develop a procedure for the determination of the K_{St} as a function of the characteristic size of the dust which does not require any chemical kinetic information (the most difficult to obtain or to recover from the literature). In this way, using a single experimental datum, that is the K_{St} value measured for the reference average diameter of the dust (particularly, the smallest one available), this methodology is able to predict the reduction of the K_{St} value when increasing the dust average diameter (starting from the reference value).

A comparison of the model predictions with several sets of experimental data involving different organic dusts showed a fair agreement, therefore strongly supporting the validity of the assumption made to develop the proposed methodology that, once further validated, could be used to strongly reduce the resources required for a complete hazard assessment when a large number of different dust mean diameter values are present in a production facility.

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Captions to the figures

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

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

Figure 3. Experimental (TG measurements carried out with a heating rate of 10 °C/min) and fitted reacting solid conversion vs. temperature data for wheat flour.

Figure 4. Characteristic time values as a function of temperature, computed for: a) wheat flour particles of 48 μm ; b) wheat flour particles of 351 μm ; c) niacin particles of 20 μm ; d) sugar particles of 300 μm .

Figure 5. Experimental data vs. model predictions.

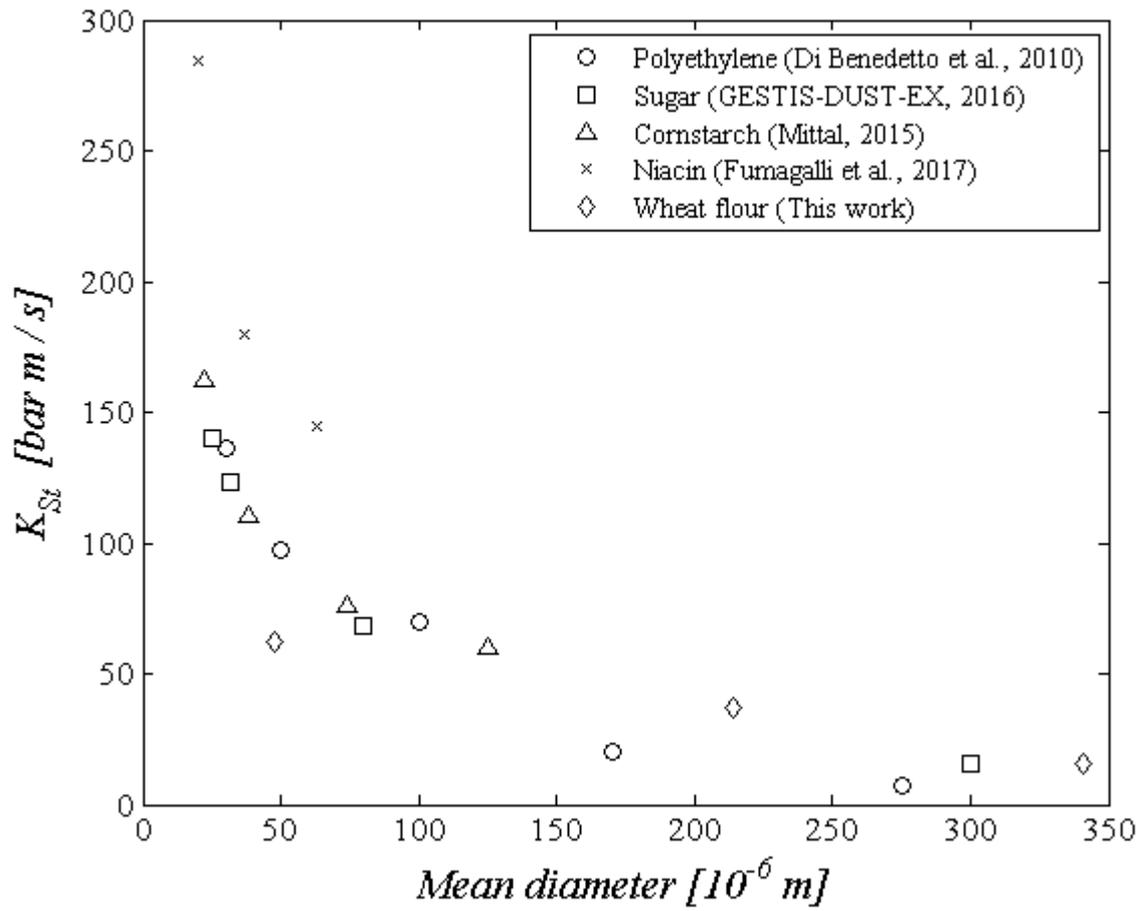


Fig. 1

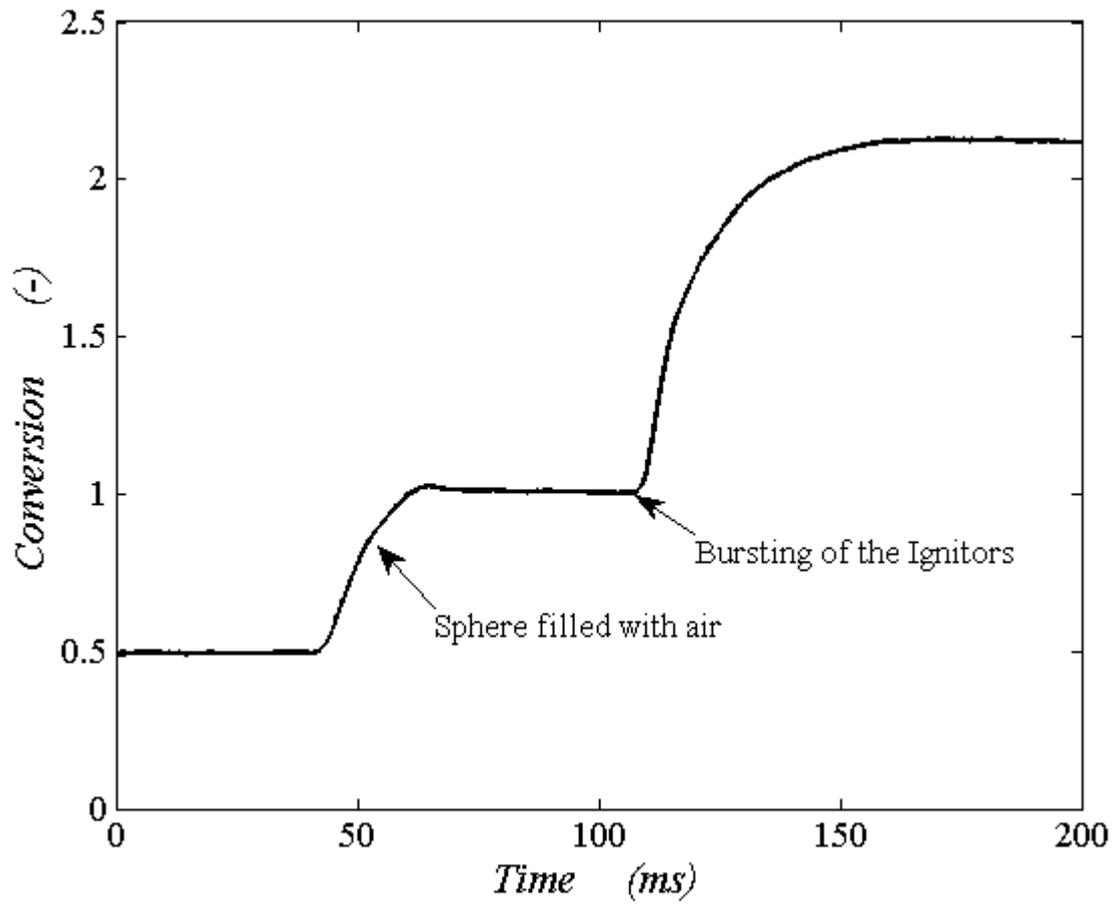


Fig. 2

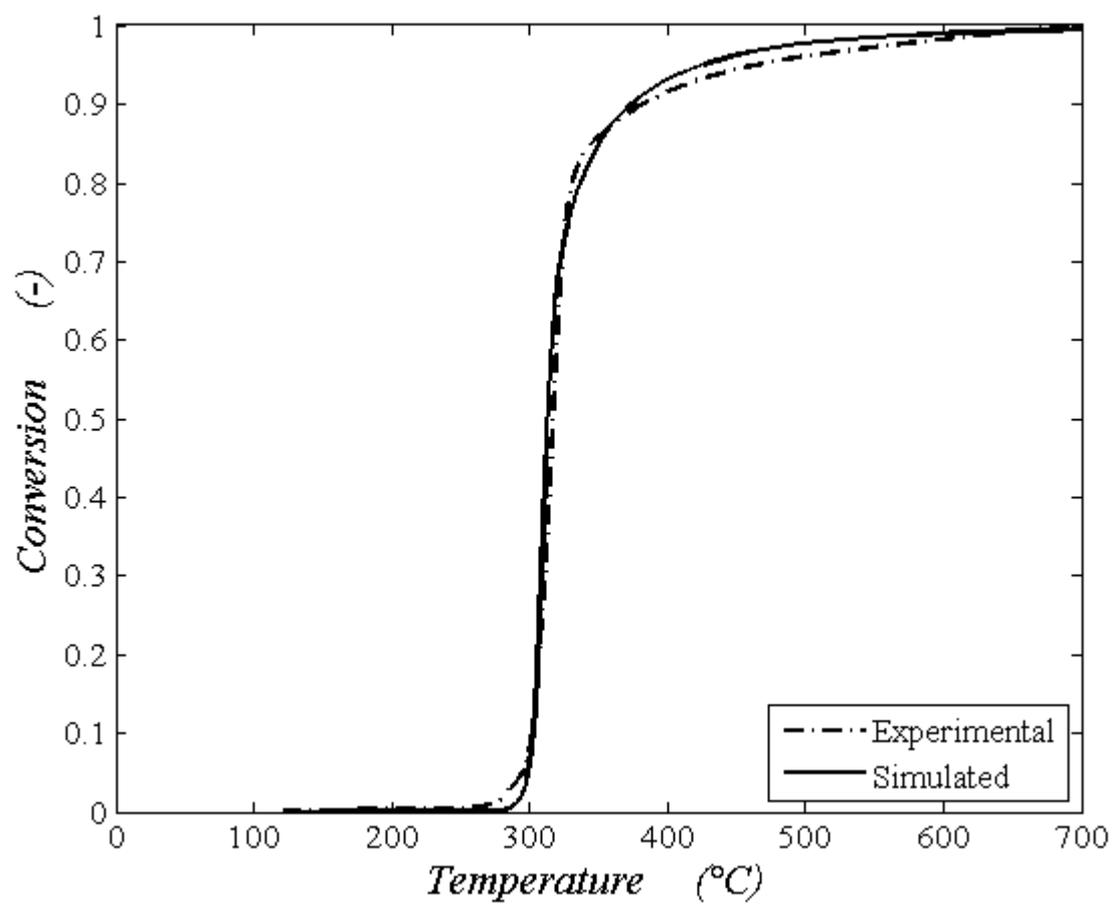


Fig. 3

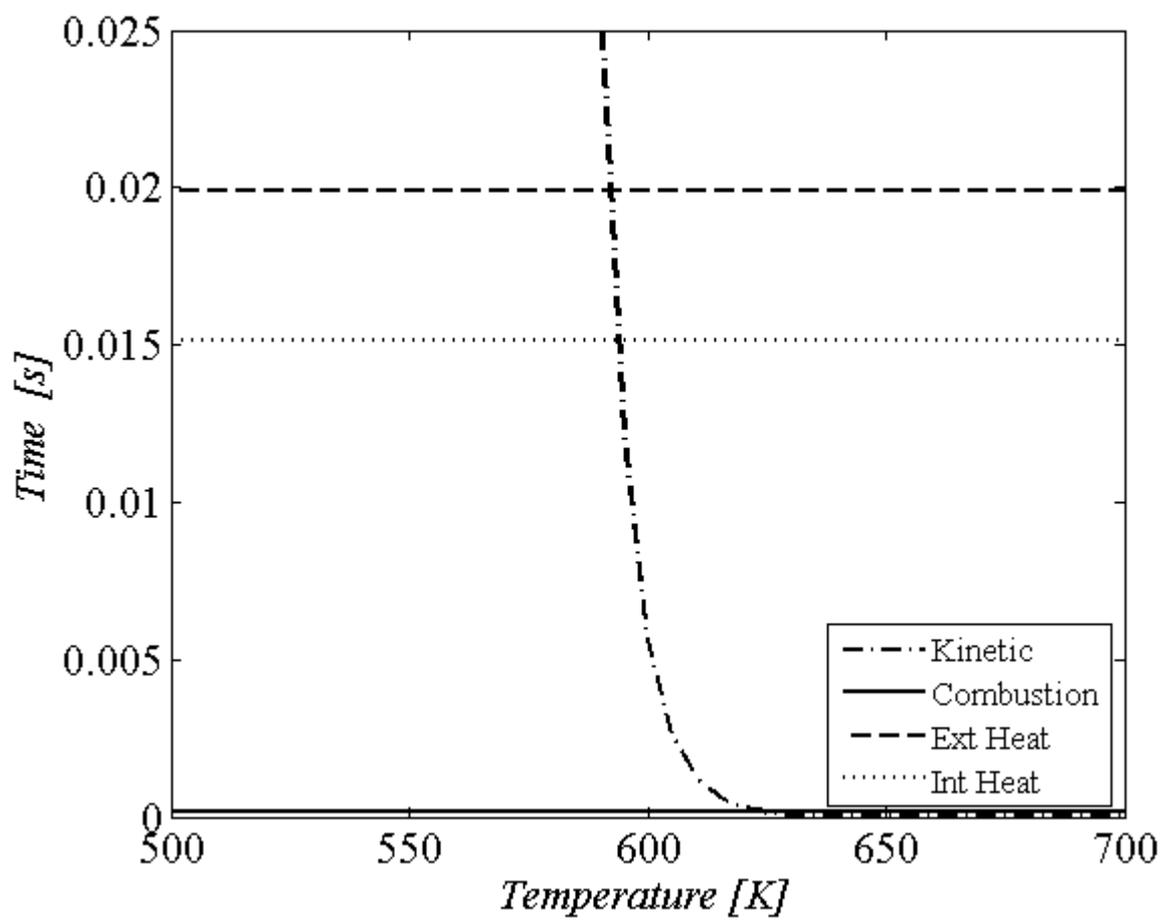


Fig. 4a

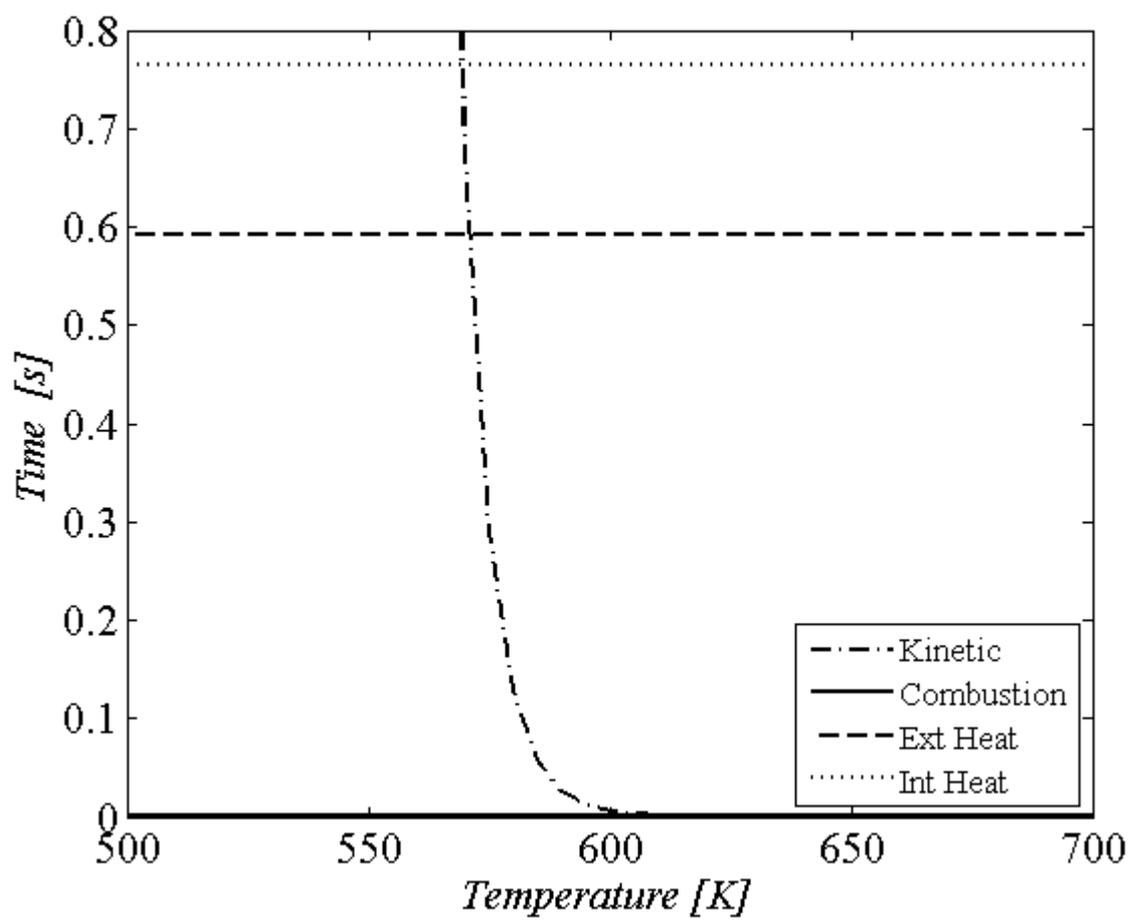


Fig. 4b

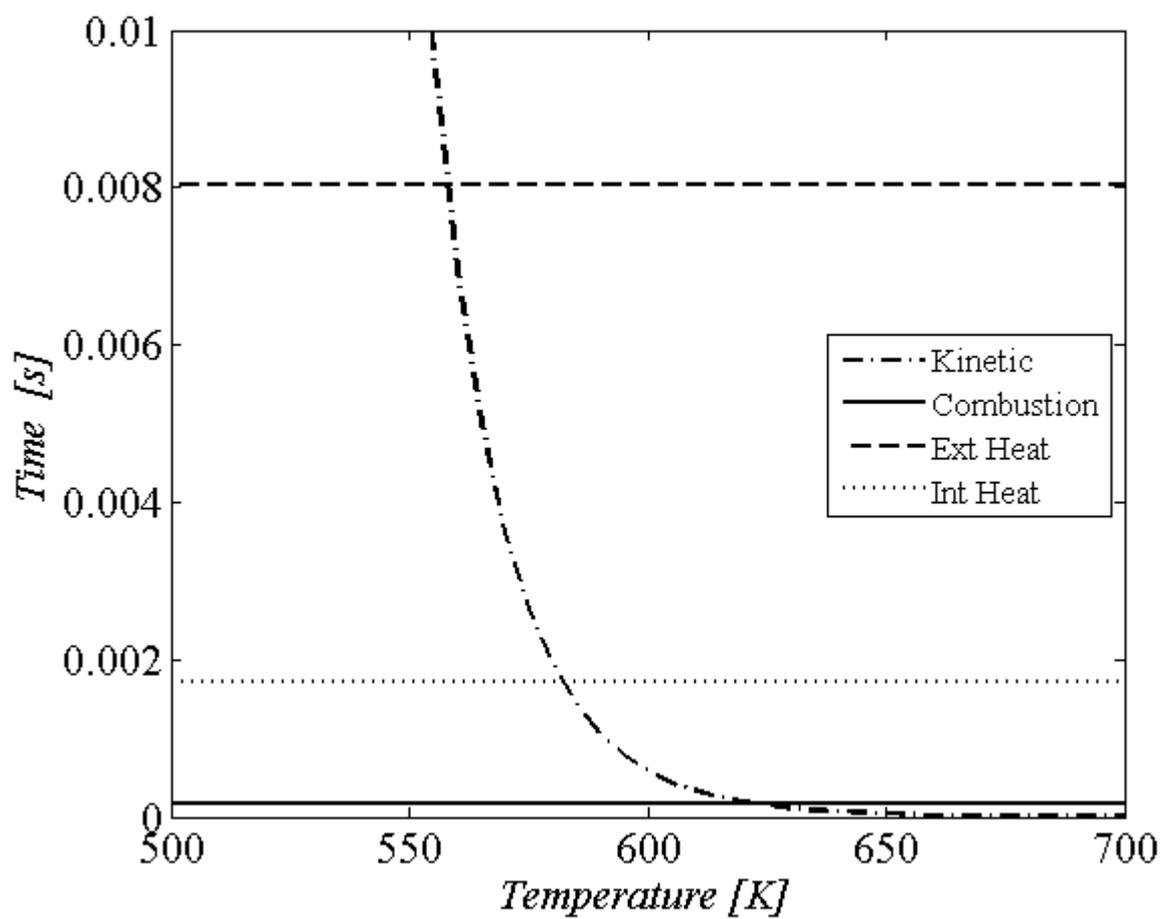


Fig. 4c

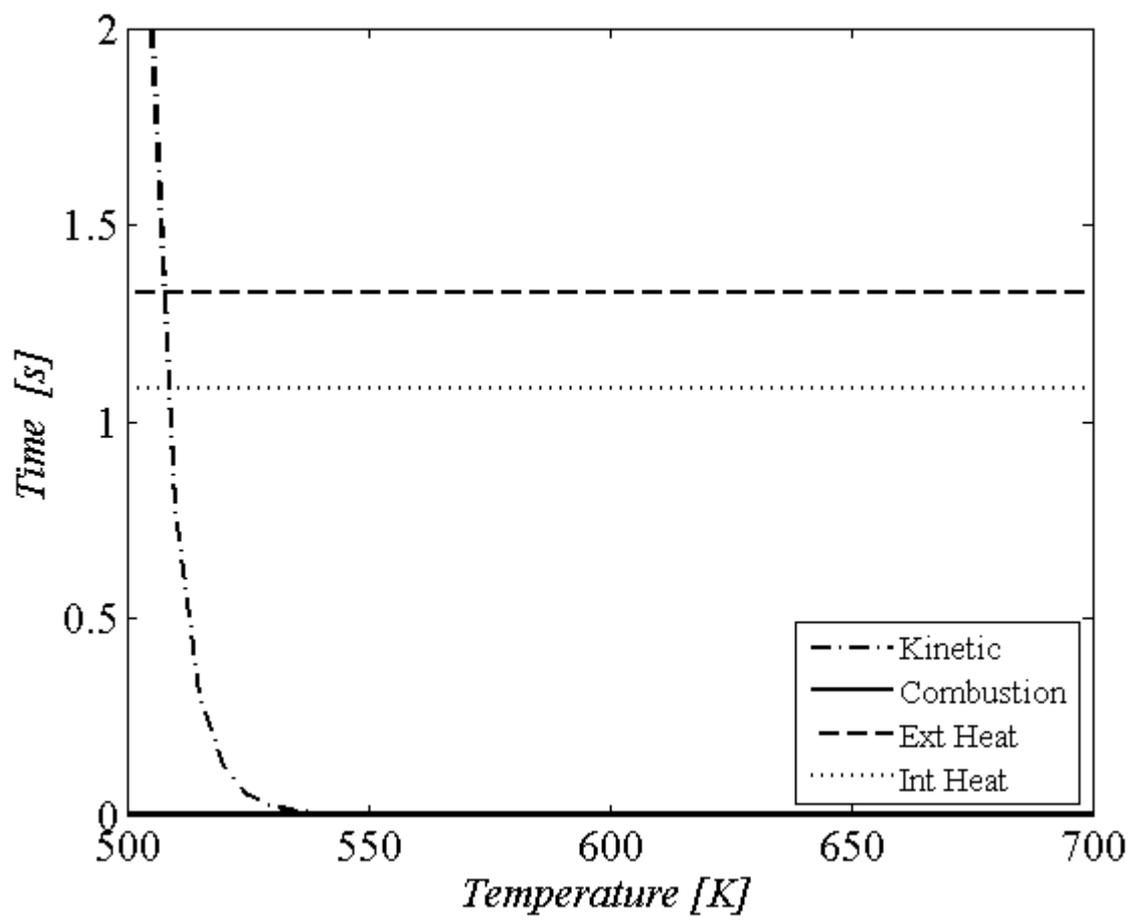


Fig. 4d

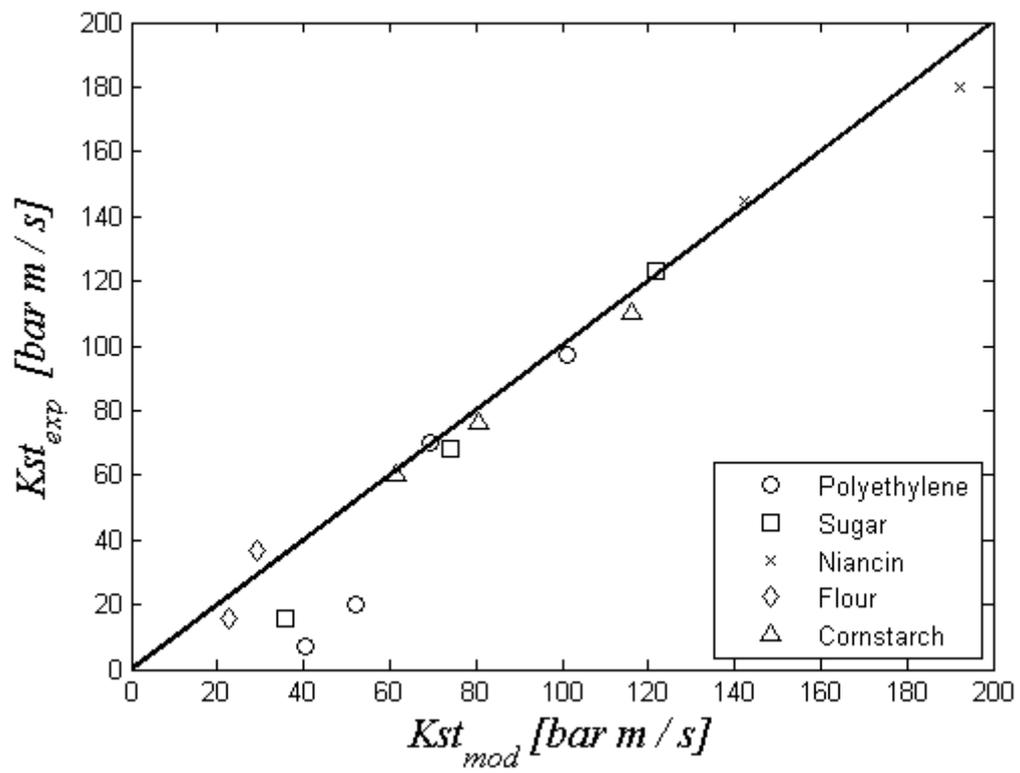


Fig. 5

TABLES

Parameter	Value
A [1/s]	1.43×10^{18}
E [J/mol]	4.53×10^5
n	9.81
χ	0.13

Table 1. Kinetic parameters values of the one-step pyrolysis reaction estimated from TG measurements for wheat flour.

Dust	Parameter	Value	References
Polyethylene	$\rho_{s,0}$ [kg/m^3]	920	Rabinovitch, 1965
	$c_{p,s}$ [$J/kg \cdot K$]	2300	Staggs, 2000
	λ [$W/m \cdot K$]	0.335	Staggs, 2000
Sugar	$\rho_{s,0}$ [kg/m^3]	1590	ICSC, 2003
	$c_{p,s}$ [$J/kg \cdot K$]	1263	Anderson et al., 1950
	λ [$W/m \cdot K$]	0.167	Maccarthy and Fabre, 1989
Niacin	$\rho_{s,0}$ [kg/m^3]	1162	Agreda, 2007
	$c_{p,s}$ [$J/kg \cdot K$]	1243	Agreda, 2007
	λ [$W/m \cdot K$]	0.335	(This work)
Cornstarch	$\rho_{s,0}$ [kg/m^3]	540	Niir Board of Consultants & Engineers, 2005
	$c_{p,s}$ [$J/kg \cdot K$]	1631	Hwang et al., 1999
	λ [$W/m \cdot K$]	0.22	Heldman, 2003
Wheat flour	$\rho_{s,0}$ [kg/m^3]	527	Berton et al., 2002
	$c_{p,s}$ [$J/kg \cdot K$]	1371	Kaletunç, 2007
	λ [$W/m \cdot K$]	0.11	Božiková, 2003

Table 2. Physical property used in the model computations.