Fire Safety Journal 61 (2013) 138–143

Contents lists available at ScienceDirect

Fire Safety Journal

journal homepage: www.elsevier.com/locate/firesaf

A linear relationship between dimensionless crossing-point-temperature and Frank–Kamenetskii reactivity parameter in self-heating test at infinite *Biot* number for slab geometry

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ARTICLE INFO

Article history:
Received 3 August 2012
Received in revised form
13 June 2013
Accepted 4 August 2013
Available online 14 September 2013

Keywords:
Self-ignition kinetics
Crossing-point temperature
Transient method
Slab geometry
Infinite *Biot* number
Frank–Kamenetskii reactivity parameter

ABSTRACT

Self-heating/ignition is one of the well-known practical causes for fires and explosions in industry and in nature. The Transient Method (or *Chen Method*) is a cost-effective approach for determining the thermal ignition parameters of packed particulate or loose materials (activation energy E, the product of the heat of reaction and the pre-exponential constant QA). The crossing-point-temperature (CPT) method to establish the ignition kinetics was initiated by the first author in 1994. A finite difference solution obtained in 1998 showed that for *Biot* number approaching infinity the dimensionless CPT, θ_{cpt} (when the conduction term becomes zero at symmetry), is proportional to the Frank–Kamenetskii reactivity parameter δ, i.e.$\theta_{cpt}=0.1\delta$. In this study, this relationship has been re-confirmed firstly by new *Matlab* simulations, and secondly, derived analytically with the characteristic transport dimension concept and a new simple idea of a three-region approximation. The dimensionless thickness of the third region (next to the solid-gas boundary), defined as $(1-\beta_2)_{self\text{-}heat}$, is remarkably similar to that for the heat conduction $(1-\beta_2)_{cond}=0.333$ which leads to $\theta_{cpt}=0.093\delta$. A small adjustment of $(1-\beta_2)_{self\text{-}heat}$ to 0.339 leads to the exact relationship. This work shows a general applicability of the approximate linear relationship, making the method more useful.

1. Introduction

There has been a sustained practical interest in self-heating/ignition related hazards over many years [1,2]. The occurrence of a fire or an explosion led by self-heating presents a huge threat to the chemical and biochemical industry. Of course self-heating/ignition may also arise in nature. A large number of theoretical studies, which have explored a great deal of the behaviours exhibited by exothermic systems have become available during the past 20 years. There has also been a series of experimental approaches that have taken the advantage of the derived solutions of the thermal ignition phenomena (especially the criticality behaviour), to measure the ignition kinetics parameters [1,3].

In 1994, Chen proposed a unique experimental procedure for measuring the thermal ignition kinetics (or kinetics parameters), which is based on the transient heating behaviour of a sample contained in a symmetrical stainless steel mesh basket. The first piece of work was carried out in an undergraduate final year project under Chen's supervision [4]. This method has been termed the Transient Method [3,4], which is sometimes also called the Chen Method [3]. This method had triggered some discussions on the kind of accuracy involved, as described by Jones [5,6]. Nevertheless, this transient approach significantly simplifies the traditional Frank–Kamenetskii procedure. Only one sample size is required at finite *Biot* number (*Bi*). This method relies on the reasonably accurate measurement of the ‘crossing-point-temperature’ T_{cpt} (the temperature at which the second derivative against distance of the geometrical centre temperature of a symmetrically heated body becomes zero) [3,7–11]. When the conduction term is zero in the differential energy balance, the rate of temperature rise is directly proportional to the reaction heat term. More details regarding this method will be reviewed later.

In one of the series of works undertaken by Chen's group at The University of Auckland, in the period between 1994 and 2006, through computer simulations, the crossing-point-temperatures for different initial temperatures of a solid slab were found to be practically the same [12]. In fact, not only were the predicted

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http://dx.doi.org/10.1016/j.firesaf.2013.08.002

Nomenclature

A	reaction frequency factor, s^{-1}
Bi	*Biot* number, dimensionless
C_p	specific heat of solid, J kg^{-1} K^{-1}
E	activation energy, J mol^{-1}
k	heat conductivity, W m^{-1} K^{-1}
Q	heat of reaction, J kg^{-1}
r_o	half-width of the slab, m
R	universal gas constant, 8.314 J mol^{-1} K^{-1}
t	time, s
T	temperature, K
x	distance from symmetry, m
z	dimensionless distance from the geometric centre

Greek symbols

α	thermal diffusivity, m^2 s^{-1}
β	Fraction of a domain defined in Fig. 3
ρ	density, kg m^{-3}
δ	Frank–Kamenetskii parameter (dimensionless)
τ	dimensionless time
θ	dimensionless temperature

Subscripts and superscripts

a	ambient or oven temperature
cpt	crossing-point-temperature (method)
o	temperature of the middle (central) region (the flat region in the two-region assumption in van der Sman's work (2007))

symmetrical temperatures the same, the temperature–distance profiles when the crossing-point-temperature occurred were also practically identical, as were the conduction-distance terms and source-term-distance profiles. However, there were exceptions (but still within several degrees Kelvin), when both the boundary conditions and initial temperatures were supercritical (supercritical conditions refer to cases in which ignitions occur in the peripheral regions rather than in the centre). Based on the calculations carried out in that study, a suggestion has been made that it may be possible to use this constant crossing-point-temperature as a physio-chemical property and as an indication of the tendency of a solid to self-ignite. This view was further strengthened by another phenomenon, illustrated through numerical simulations by Chen and Chong [12] for the infinite slab geometry. They showed that that the dimensionless temperature at the crossing-point θ_{cpt} is proportional to the Frank–Kamenetskii parameter δ [1]. The numerical simulations were conducted for the case where $Bi \rightarrow \infty$ for δ values from 0 to 1.2 and the proportionality was 0.10. This numerical result has been re-confirmed in this work using independent *Matlab* simulations.

The above is an important finding, which can help further reduce the effort required for thermal ignition testing. The problem is that the general applicability of this result is vague. Since 1998, after the publication of the paper by Chen and Chong [12], Chen has also attempted, many times, to seek a way to illustrate this result analytically without success. An analytical illustration of this linear relationship between θ_{cpt} and δ is provided in this work.

2. Transient method (TM) for measuring thermal ignition kinetics

To date, the most widely used standard test has been the Frank–Kamenetskii method which is based on the steady state analysis established many years ago. Details of this approach can be found in many previous publications [1,12]. The transient method (TM) was initiated by Chen in 1994 [4] and in the same laboratory extensive experimental works were conducted to establish the ignition kinetics of packed powder materials (dairy powders, wood sawdust etc.) [3,7–11,13]. Chen and Chong [12] also numerically demonstrated some interesting characteristics of the 'cross-over' phenomenon. This 'cross-over' phenomenon was first pointed out by Gray [14,15], was the foundation for the experimental cross-point temperature (CPT) method. They attributed such a phenomenon to the existence of peripheral heating (see Fig. 1(a) and (b)). In 1994, Chen figured out that such phenomenon could be taken advantage of by devising a new ignition kinetics measurement, i.e. the crossing-point temperature (CPT) method as it was called at the time. This approach was later adopted by other researchers at the University of Adelaide, Australia [16], University of California, Berkeley, United States [17], Leeds University, United Kingdom [18,19], and Central South

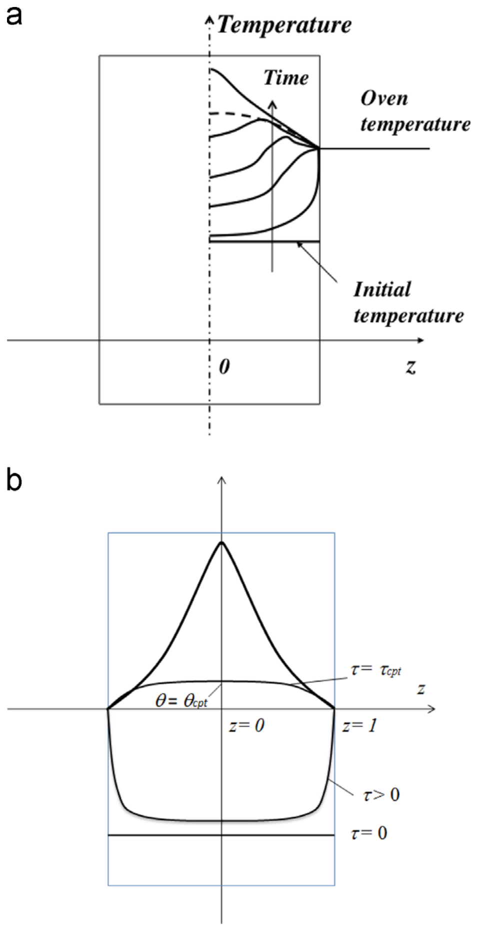

Fig. 1. Evolution of an exothermic reaction in an infinite slab heated on both sides with the same boundary condition ($Bi \rightarrow \infty$). (a) Dimensional profiles and (b) dimensionless profiles. The figures show the transition of the temperature from below the crossing-point (cross-over) temperature (*cpt*) to above it.