Fire Research Note No. 842

THERMAL EXPLOSION IN RECTANGULAR PARALLELEPIPEDS

by

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SUMMARY

The Frank-Kamenetskii thermal explosion parameter, δ_c , is calculated for rectangular parallelepipeds with sides in the ratio of 1 : p : q. It is given by:-

$$\delta_c = 0.873\ (1 + 1/p^2 + 1/q^2)$$

The coefficient includes a small correction to give agreement to within 1 per cent of existing values of δ_c for the extreme configurations, i.e. the cube when p = q = 1 and the infinite plane slab when $p = q = \infty$.

KEY WORDS: Thermal explosion, self-heating, parallelepipeds

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JOINT FIRE RESEARCH ORGANIZATION

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INTRODUCTION

In applying the thermal explosion model to problems of self-heating and ignition in materials stored in the form of rectangular piles (e.g. stacked bags) it is necessary, when approximation by a cube is inappropriate, to evaluate the Frank-Kamenetskii thermal explosion parameter for the general case of the rectangular parallelepiped. In spite of its practical utility, the calculation for this general case does not so far appear to have been published. An approximate calculation is given in this note.

CALCULATION

The calculation, which follows below, is a straightforward application of established approximate procedures[1,2] for self-heating in solids due to a single reaction which is effectively of zero order and which shows Arrhenius temperature dependence.

Using the "effective transfer coefficient" approximation, the Frank-Kamenetskii equation for self heating in a solid can be written as:

$$\frac{d\theta}{d\tau} = \delta e^{\theta} - \tau \frac{S}{V} \beta \theta \qquad (1)$$

where

θ = dimensionless temperature increase at the centre of the solid (above a constant surface temperature)

τ = dimensionless time = kt/r^2

k = thermal diffusivity

t = time

S = surface area of solid

V = volume of solid

β = effective transfer coefficient (dimensionless)

δ = Frank-Kamenetskii self-heating parameter (dimensionless) r is a length which, for the rectangular parallelepiped and in conformity with standard usage in thermal ignition theory, is taken as half the length of the shortest side.

The critical value of δ, δ_c, is given by

$$\delta_c = rS\beta/Ve \qquad (2)$$

Following Frank-Kamenetskii[1] and Thomas[2] the heat transfer term in equation (1), $rS\beta/V$, is evaluated by comparison with the quasi-stationary equation for conduction as follows.

From the more general solution given by Carslaw and Jaeger[3] it may be shown that the central temperature in a rectangular parallelepiped with sides a, b and c, initially at a uniform temperature, θ_i (>0), is given by

$$\frac{\theta}{\theta_i} = \frac{64}{\pi^3} \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{lmn} \sin\frac{l\pi}{2} \sin\frac{m\pi}{2} \sin\frac{n\pi}{2} \times \exp\left\{ - k\pi^2 t \left[\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2} \right] \right\}$$

for integers l, m and n all odd. (k = thermal diffusivity).

In the quasi-stationary state, i.e. when t is large, only the first term, $l = m = n = 1$, is important. Then, we have

$$\frac{d\theta}{d\tau} = -\frac{\pi^2}{4} \left(1 + \frac{a^2}{b^2} + \frac{a^2}{c^2}\right) \theta \qquad (3)$$

Comparing equation (1) for an inert solid ($\delta = 0$) with equation (3) we have

$$r\,S\beta/V = \frac{\pi^2}{4} \left(1 + \frac{a^2}{b^2} + \frac{a^2}{c^2}\right),$$

whence, from equation (2),

$$\delta_c = \frac{\pi^2}{4e} \left(1 + \frac{1}{p^2} + \frac{1}{q^2}\right) \qquad (4)$$

where $p = b/a$, $q = c/a$.

The extreme values of δ_c given by equation (4) correspond to the cube, $p = q = 1$, and the infinite plane slab, $p = q = \infty$, and are compared with accepted values from other sources in Table 1.

Table 1

Extreme values of δ_c in equation (4)

Configuration	equation (4)	Literature	corrected
Infinite slab	0.908	0.88*	0.87
cube	2.73	2.60**	2.62

* Frank-Kamenetskii[1]

** Parks[4], value selected for $30 \leqslant E/RT_A \leqslant 80$ (where, as usual, E = activation energy, R = gas constant, T_A = ambient temperature)

Reducing the values given by equation (4) by 4 per cent yields the corrected values in the final column of Table 1, which are within about 1 per cent of the literature values.

With this correction, equation (4) becomes

$$\delta_c = 0.873 \left(1 + \frac{1}{p^2} + \frac{1}{q^2}\right) \qquad (5)$$

COMMENTS

For convenience, equation (5) is plotted in Fig. 1 and the positions of a range of parallelepipeds ~~is~~ are indicated. On the basis of this calculation, the value of $\delta_c = 2.94$ which has been quoted[5] for the parallelepiped 1 : 1 : 2 is incorrect; it is, in fact, outside the possible range.

From inspection of Fig. 1, it will be seen that δ_c decreases markedly for quite a moderate departure from cubic symmetry; e.g. for the parallelepiped with sides 1 : 4/3 : 4/3 , δ_c is 37 per cent less than the value for the cube.

The parallelepiped with sides 1 : 5 : 5 has a value of δ_c only about 6 per cent higher than for the infinite slab and supports an earlier empirical conclusion[6] that a slab of diameter five or more times its thickness could be treated as having infinite extent.

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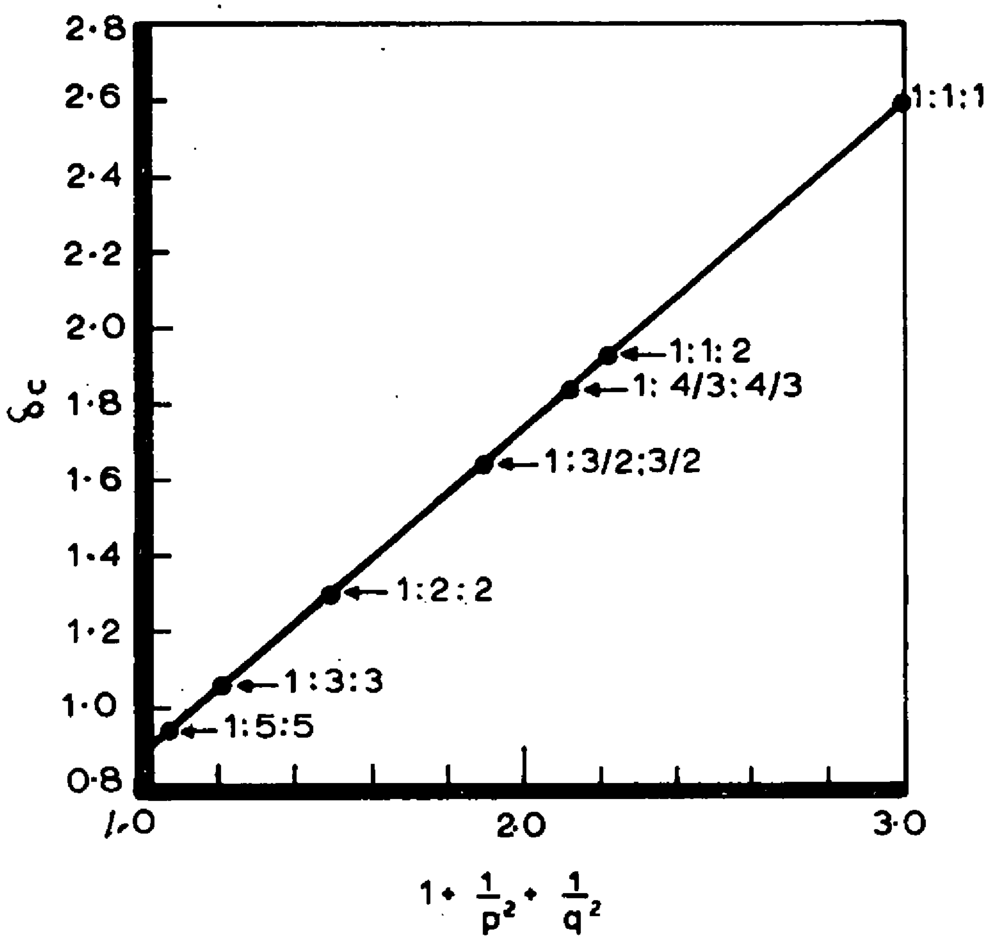

FIG. 1 CRITICAL EXPLOSION PARAMETER FOR RECTANGULAR PARALLELEPIPEDS WITH SIDES 1 : p : q