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THERMAL EXPLOSION IN THE SHORT CYLINDER WITH A GENERAL BOUNDARY CONDITION

by

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SUMMARY

Approximate expressions are obtained for the critical explosion parameter and critical temperature rise for thermal explosion in a short cylinder of material of finite conductivity and with a finite surface heat transfer coefficient.

MINISTRY OF TECHNOLOGY AND FIRE OFFICES' COMMITTEE
JOINT FIRE RESEARCH ORGANIZATION

LIST OF SYMBOLS

A	Pre-exponential factor of Arrhenius equation.
a	Thermal diffusivity.
D	Diameter of cylinder.
E	Activation energy in Arrhenius equation.
h	Average surface heat transfer coefficient for all surfaces of cylinder.
K	Thermal conductivity.
L	Length of cylinder.
l	Half-length of cylinder.
m	x/r
n	z/l
Q	Heat of reaction per unit mass.
r	Radius of cylinder.
T	Temperature, $^{\circ}K$, subscripts o, s, A, refer to centre, surface and ambient respectively.
t	Time
x	Distance along radius.
z	Distance along half-length.
α	hr/K, dimensionless.
β	Effective heat transfer coefficient, dimensionless.
δ	Explosion parameter, defined for equation (1).
θ	Dimensionless temperature, defined for equation (1).
τ	Fourier number, equation (1)
ρ	Density.

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INTRODUCTION

In experimental studies of thermal explosion in explosives and unstable compounds it is usually most convenient to study samples in the form of short cylinders.

The critical parameter of the stationary state model for thermal explosion in a short cylinder of material of finite conductivity has been calculated by Frank-Kamenetskii[1] for a boundary condition which assumes an infinite surface heat transfer coefficient. In practice, however, one is commonly concerned with explosion in cylinders of small size for which the effect of a finite surface heat transfer coefficient cannot properly be ignored.

This note extends the approximate procedure of Frank-Kamenetskii[1] and Thomas[2] to a calculation of the critical explosion parameter for a short cylinder with a general boundary condition. Certain other results pertinent to the experimental study of the explosion of short cylinders are also obtained.

THEORETICAL

Self-heating equation

With heat generation due to a zero order reaction obeying the Arrhenius equation, the equation for self-heating in the finite circular cylinder $0 < x < r$, $-l < z < l$ (diameter $D = 2r$ and length $L = 2l$) takes the form

$$\frac{\partial^2\theta}{\partial m^2} + \frac{1}{m}\frac{\partial\theta}{\partial m} + \frac{r^2}{l^2}\frac{\partial^2\theta}{\partial n^2} = \frac{\partial\theta}{\partial\tau} - \delta e^{\theta} \qquad (1)$$

when the exponential approximation[1] for the Arrhenius term is used and the following dimensionless variables are introduced:-

$$\theta = \frac{E}{RT_A^2}(T - T_A),$$

$$m = x/r, \quad n = z/\underline{l}$$

$$\tau = at/r^2$$

$$\delta = \frac{E}{RT_A^2}\frac{\rho r^2}{K} QAe^{-E/RT_A}$$

In order to introduce a general boundary condition, it is convenient to introduce an <u>average</u> heat transfer coefficient, h, for all surfaces of the cylinder and an <u>average</u> surface temperature, T_s. The boundary condition may then be written

$$\frac{d\theta}{dm} = -\alpha\theta_s \quad \text{at } m = 1,$$

$$\frac{d\theta}{dn} = -\alpha\frac{l}{r}\theta_s \quad \text{at } n = \pm 1,$$

where

$$\alpha = hr/K \text{ and } \theta_s = \frac{E}{RT_A^2}(T_s - T_A)$$

The remaining conditions are:-

$$\frac{d\theta}{dm} = 0 \text{ at } m = 0, \quad \frac{d\theta}{dn} = 0 \text{ at } n = 0$$

and

$$\theta = 0 \text{ when } \tau = 0$$

For thermal explosion, we require the maximum value of the function $\delta(\alpha, D/L)$, denoted δ_c, for which a steady state solution to equation (1) can exist. This may be found by the method of Frank-Kamenetskii[1] and Thomas[2] in which the conduction terms in equation (1) are replaced by a term involving an effective heat transfer coefficient. The equation then becomes

$$\frac{d\theta_o}{d\tau} = \delta e^{\theta_o} - r\frac{S}{V}\beta\theta_o \qquad (2)$$

where θ_0 is the dimensionless centre temperature, β is the dimensionless effective heat transfer coefficient and $\frac{S}{V}$ is the surface to volume ratio which, for the finite cylinder, is $2\ (L + r)/rL$.

In the steady state the maximum or critical, value of δ in equation (2) corresponds to $\theta_0 = 1$ and is given by

$$\delta_c = \frac{2}{e}\,\frac{L + r}{L}\beta \ . \tag{3}$$

β is evaluated by inserting the quasi-stationary solution (τ large) of the exact conduction equation for the inert cylinder (equation (1) with $\delta = 0$) with, in this case, a radiation boundary condition[3] into equation (2) with $\delta = 0$.

Comparison with equation (3) then gives

$$\delta_c = \frac{1}{e}\left\{\mu^2 + (\gamma\frac{D}{L})^2\right\} \tag{4}$$

where γ is the first root* of

$$\gamma \tan\gamma = \alpha\, D/L$$

and μ is the first positive root* of

$$\mu J_1\ (\mu) = \alpha J_0\ (\mu)$$

where J_1 and J_0 are Bessel functions of the first kind and of first and zero order respectively.

When $\alpha = \infty$, equation (4) reduces to the equation obtained by Frank-Kamenetskii[1], who found that the above procedure tends to give values of δ_c about 8 per cent higher than those which can be obtained analytically for certain geometries without approximation of the conduction terms. Accordingly, values of δ_c calculated from equation (4) may be reduced by 8 per cent for consistency with the latter results.

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*Roots of these equations are tabulated in Reference 3.

Critical temperature rise

The above procedure does not provide a satisfactory estimate for the critical temperature rise; thus, it gives a value 40 per cent too low for the infinite cylinder when $\alpha = \infty$. This temperature rise is better estimated by a comparative method due to Wake and Walker[4]. Extending their approach to the comparison of critical temperature increases at a given ambient temperature, and using the approximate proportionality of the α correction for different geometries as recently justified by Merzhanov[5], we have, in the notation of the present paper,

$$\theta_o(\alpha)_{\text{cylinder}} \doteq \frac{6}{4}\, \theta_o(\alpha)_{\text{sphere}} \times N_1 \left(\frac{L}{D}\right) \frac{\delta_c(\infty, L/D)\ \text{cylinder}}{\delta_c(\infty)\ \text{sphere}} \qquad (5)$$

where N_1 (L/D) is a function calculated by Wake and Walker for the finite cylinder with heat generation at a rate independent of temperature, and $\theta_o(\alpha)_{\text{sphere}}$ is the critical temperature rise in a sphere, at given α, for a reaction obeying the Arrhenius equation[6]. For an infinite cylinder with $\alpha = \infty$, the estimate of the critical value of θ_o given by equation (5) is five per cent higher than the value given by solution of the self-heating equation with a reaction rate governed by the Arrhenius equation. Having obtained an estimate of the critical value of θ_o, sub-critical values corresponding to any $\delta/\delta_c < 1$ at given α can be estimated by the method of Thomas and Bowes[7]. This method may be expected to yield reasonable estimates for sub-critical θ_o for any completely bounded solid with a surface to volume ratio similar to that of a sphere.

Estimation of α

From a consideration of the heat balance between the cylinder and its surroundings in a sub-critical steady state, it is seen that, for the effective transfer approximation, (see also Thomas's second approximation method[2])

$$\alpha\ (T_s - T_A) = \beta_\infty (T_o - T_s) = \beta\ (T_o - T_A) \quad ;$$

whence

$$\alpha = \beta_\infty \frac{T_o - T_s}{T_s - T_A} \qquad (6)$$

where β_{∞} is the value of β at $\alpha = \infty$ and is calculated from equation (7) by inserting the value of δ_c for $\alpha = \infty$. For a cylinder having $L/_D = 1.6$, as used in a study of thermal explosion in peroxides (to be reported elsewhere), this value of δ_c is 2.33 and β_{∞} is 2.42. Equation (6) provides a convenient way of estimating α from experimental measurements under nearly-stationary conditions, i.e. in the neighbourhood of a temperature maximum or pre-explosion inflexion in the temperature record for a self-heating system.

REFERENCES

1. FRANK-KAMENETSKII, D. A. "Diffusion and heat exchange in chemical kinetics". Translated N. Thon, Princeton University Press, Princeton 1955.
2. THOMAS, P. H. Some approximations in the theory of self-heating and thermal explosion. Trans. Faraday Soc., 1960, 56, 833.
3. CARSLAW, H. S. and JAEGER, J. C. "Conduction of heat in solids". Clarendon Press, Oxford, 2nd Edition 1959. p. 227.
4. WAKE, G. C. and WALKER, I. K. Calorimetry of oxidation reactions. N.Z. J. Sci. 1964, 7, 227.
5. MERZHANOV, A. G. Problems of heat transfer in the theory of thermal explosion. Proc. All-Union Conference on Heat and Mass Transfer. Minsk, 5-9th May, 1964.
6. THOMAS, P. H. On the thermal conduction equation for self-heating materials with surface cooling. Trans. Farad. Soc. 1958 54, Part I, 60.
7. THOMAS, P. H. and BOWES, P. C. Some aspects of self-heating and ignition of solid cellulosic materials. Brit. J. Appl. Phys., 1961, 12, 222.