SOME VARIATIONAL PROBLEMS IN THERMAL EXPLOSION THEORY

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Many of the results obtained in the stationary theory of thermal explosion relate to symmetrical regions in which the temperature distribution depends on a single space coordinate. Important practical problems with two or three independent variables lead to nonlinear partial differential equations, whose solution involves serious mathematical difficulties. In [1] a variational method was proposed for such problems. However, in the formulation adopted in [1] obtaining numerical results requires laborious calculations. Consequently, in [1] the only value obtained by a variational method is that of the critical parameter for a sphere, which differs by 25% from the known exact solution. The computational difficulties encountered in solving the above-mentioned variational problems are associated with the form of the relation between heat release and temperature in the heat conduction equation and can be eliminated by choosing another more convenient approximation of the Arrhenius law for temperatures $T \ll E/R$ (E is the activation energy).

We note that the actual heat release corresponding to an exothermic chemical reaction will be a bounded function of temperature. Hence it follows that there always exists at least one solution of the corresponding stationary heat conduction problem. However, in the theory of thermal explosion only those solutions corresponding to low (as compared with E/R) temperatures are of physical interest. In this temperature region the boundedness of the heat release still has no effect, so that replacing the bounded source with one that increases without bound[1] leads only to the nonexistence of a high-temperature solution, which at high activation energies is of no interest.

Evidently, it is simplest and most convenient to approximate the function exp (−E/R) in the region $RT \ll E$ by a quadratic trinomial, as proposed in [2]. The expression given in [2] is valid at $RT/E \sim 10^{-2}$. The region of applicability of this approximation can be extended somewhat. We introduce the relation

$$\exp\frac{-E}{RT} \approx \exp\frac{-1}{\alpha}\,[1 + A(\alpha)\theta + B(\alpha)\theta^2],$$
$$\left(\theta = \frac{T - T_0}{\alpha T_0},\quad \alpha = \frac{RT_0}{E}\right). \tag{1}$$

Here T_0 is the temperature at the boundary. The coefficients A, B must be so selected that (1) is the best approximation on the interval $0 \le \theta \le 2.5$, which is alone of interest in the theory of thermal explosion. Below we present values of $A(\alpha)$ or $B(\alpha)$ for several values of α. The last column also gives the coefficients from [2] determined so that the approximation is the best in the neighborhood of the point $\theta = 1$.

α=0.01	0.05	0.10	0
A=0.309	0.650	0.825	0.718
B=1.412	0.988	0.667	1.000.

The error of approximation (1) does not exceed about 3%.

Keeping in mind the described approximation, we will consider the boundary value problem in the region D

$$\Delta\theta + qF(\theta) = 0,\quad \theta\,|\,\Gamma = 0\quad F(\theta) = 1 + A\theta + B\theta^2,$$
$$\Delta = \frac{\partial^2}{\partial\xi^2} + a\frac{\partial^2}{\partial\eta^2} + b\frac{\partial^2}{\partial\zeta^2},\quad \xi = \frac{x}{l_1},\quad \eta = \frac{y}{l_2},\quad \zeta = \frac{z}{l_3},$$
$$a = \left(\frac{l_1}{l_2}\right)^2,\quad b = \left(\frac{l_1}{l_3}\right)^2,\qquad q = \frac{l_1^2 Q}{4\lambda T_0\alpha}\exp\frac{-1}{\alpha}. \tag{2}$$

Here l_1, l_2, l_3 are the greatest dimensions of the region B along the x, y, z axes respectively. We write the variational principle corresponding to problem (2) in the form

$$\delta I = \delta\int_{(D)}\left[\theta_\xi^2 + a\theta_\eta^2 + b\theta_\zeta^2 - 2q\left(\theta + \frac{A}{2}\theta^2 + \frac{B}{3}\theta^3\right)\right]dV = 0. \tag{3}$$

We will first consider problem (2) for the interval $0 \le \xi \le 1$; its solution will be required in what follows. The temperature distribution can be written in the form

$$(1-\xi)\,q^{1/2} = \left(\frac{2c}{1 + Ac + Bc^2}\right)^{1/2}\int_v^1 \frac{du}{(1 - k_1u^2 + k_2u^4)^{1/2}}$$
$$v = (1 - \theta/c)^{1/2}. \tag{4}$$

Here $c = \theta(0)$ is a constant of integration determined from the relation

$$q^{1/2} = \left(\frac{2c}{1 + Ac + Bc^2}\right)^{1/2}\int_0^1 \frac{du}{(1 + k_1u^2 + k_2u^4)^{1/2}},$$
$$k_1 = \frac{c\,(^1/_2A + Bc)}{1 + Ac + Bc^2},\qquad k_2 = \frac{^1/_3Bc^2}{1 + Ac + Bc^2}. \tag{5}$$

Henceforth, for definiteness, in obtaining numerical results we will take the values A = 0.72 and B = 1. Simple calculations show that (5) can be solved for c at $q \le q^* = 0.88$; the corresponding value $c^* = 1.20$. These results coincide with those obtained in [4].

We now return to the functional (3). Using the known theorem of the calculus of variations [5], we can show that the function $\theta(\xi)$, determined from (4), gives a minimum value of the functional (3). Selecting the simplest trial function

$$\theta(\xi) = c\,(1 - \xi^2) \tag{6}$$

with parameter c, after substitution in (3) we obtain a quadratic equation for c, which has real roots only at $q \le q^* = 0.89$; the corresponding $c^* = 1.21$, which is very close to the exact values. The critical values for a sphere and a cylinder thus obtained are respectively equal to: $q^* = 3.63$, $c^* = 1.61$ (sphere) and $q^* = 2.11$, $c^* = 1.41$ (cylinder). These values are also close to the exact values, somewhat exceeding them. In the general case it is not possible to show that values of q^* obtained as the condition of solvability of a certain system of algebraic equations following from (3) will always exceed the exact values.

We will now consider the problem for a cylinder of finite length. The simplest trial function $\theta(\rho, \xi) = c(1 - \rho^2)(1 - \xi^2)$ gives

$$q^* = 2.14\,b + 0.88, \tag{7}$$

for a rectangle (with $\theta(\xi,\eta) = c\,(1 - \xi^2)(1 - \eta^2)$)

$$q^* = 0.87\,(1 + a), \tag{8}$$

for a parallelepiped ($\theta(\xi,\eta,\zeta) = c\,(1 - \xi^2)(1 - \eta^2)(1 - \zeta^2)$)

$$q^* = 0.85\,(1 + a + b). \tag{9}$$

The dependence of q^* on the parameters a and b in (7), (8), (9) is associated with a particular form of the trial function. More exact results can be obtained by using the method of L. V. Kantrovich [3]. In the case of a rectangle we set $\theta(\xi, \eta) = (1 - \eta^2) \times f(\xi)$. We will assume that $a = (l_1/l_2)^2 \leqslant 1$ (otherwise ξ and η must be transposed). Substituting in (3) and integrating with respect to η, we arrive at a one-dimensional variational problem with a Euler equation in the form

$$f'' + q\,(1.25 + 0.72f + 0.71f^2) - 2.50\,af = 0. \tag{10}$$

This is the equation of the one-dimensional problem (2), which is solvable if an equation of type (5) for the constant of integration is

[1]More correctly, increasing more rapidly than a linear function of temperature.

solvable. Similarly for a cylinder of finite length we set $\theta(\rho, \xi) = (1 - \rho^2) f(\xi)$. The equation for $f(\xi)$ has the form

$$f'' + q(1.50 + 0.72 f + 0.75 f^2) - 6bf = 0 \qquad (b = l_1 / R). \quad (11)$$

Here R is the radius of the cylinder. Below we present values of q^* for a rectangle calculated from the solution of (8) and (10) at different values of a, together with values of q^* for a cylinder calculated in accordance with (7) and (11) at different values of b.

a	$q^*_{(8)}$	$q^*_{(10)}$	b	$q^*_{(7)}$	$q^*_{(11)}$
0.045	0.91	0.89	0.052	0.99	0.95
0.21	1.05	1.03	0.13	1.16	1.12
0.35	1.18	1.16	0.34	1.60	1.54
0.77	1.55	1.55	1.29	3.60	3.49

REFERENCES

1. A. M. Grishin, "Some problems of ignition theory," PMTF, no. 5, 1962.
2. P. Gray and M. J. Harper, The Thermal Theory of Induction Period and Ignition Delays. Seventh Symp. (Internat.) on Combustion, Butterworths Sci. Publ., Lnd., p. 425, 1959.
3. L. V. Kantorovich and V. I. Krylov, Approximate Methods of Higher Analysis [in Russian], Fizmatgiz, 1962.
4. D. A. Frank-Kamenetskii, Diffusion and Heat Transfer in Chemical Kinetics [in Russian], Izd-vo AN SSSR, 1947.
5. I. M. Gel'fand and S. V. Fomin, Calculus of Variations [in Russian], Fizmatgiz, 1961.

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