CALCULATION OF THE CRITICAL CONDITIONS FOR A THERMAL EXPLOSION IN AN INHOMOGENEOUS MEDIUM BY A METHOD OF INTEGRAL RELATIONS

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UDC 536.46

We develop a method of integral relations for problems of thermal explosion. We find the condition for ignition of a turbulent reactive stream in a pipe.

The critical values of the parameters $\delta = \delta_*$ (the critical condition for thermal explosion) at which the solution of the boundary-value problem

$$\xi^{-n} d(\xi^n f(\xi)\, d\theta/d\xi) + \delta\varphi(\theta) = 0; \tag{1}$$

$$\xi = 0 \quad d\theta/d\xi = 0; \quad \xi = 1 \quad d\theta/d\xi = -\mathrm{Bi}\theta; \tag{2}$$

$$\varphi(\theta) = \exp(\theta), \tag{3}$$

ceases to exist have been determined analytically (for $f(\xi) \equiv 1$) for a number of special cases [1, 2]. To find δ_* in general form one can use numerical methods or approximate estimates [1, 3, 4].

Among the approximate methods for estimating $\delta_*(n, \mathrm{Bi})$ we may note Khudaev's method [5], which yields a reliable upper bound. In using this method, we must find the first eigenvalue of the appropriate boundary-value problem, which in the general case of an inhomogeneous medium $f(\xi) \not\equiv 1$ is not always possible. If $f(\xi) \not\equiv 1$, severe difficulties also arise in the use of the variational method [6].

The most acceptable method for estimating δ_* in an inhomogeneous medium is probably the method of integral relations [7], which has been used previously [8] for finding critical conditions. The accuracy of this method is determined to a great extent by a successful choice of the total profile of temperature.

In the present study we propose the development of a method of integral relations for problems in thermal explosion.* First, we give a method for choosing the temperature trial profile. Second, we consider a procedure for obtaining integral relations which is less sensitive to errors in the choice of the trial function than those used in [8].

To illustrate and confirm the method, we use the example of a classical problem of thermal explosion in a homogeneous medium. For convenience in calculations, instead of (3) we shall hereafter use the Gray – Harper approximation [9]:

$$\varphi(\theta) = \exp(\theta) \approx 1 + \gamma\theta + \theta^2, \qquad \gamma = e - 2 \approx 0.72. \tag{4}$$

1. Determination of the critical conditions for $f(\xi) \equiv 1$. As the trial profile, we select the solution of the heat-conduction equation with a constant source:

$$\xi^{-n} d(\xi^n d\theta/d\xi) + \delta = 0$$

with the boundary conditions (2). We write this solution in the form

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*In the article we use D. A. Frank-Kamenetskii's dimensionless variables: n reflects the geometry of the vessel, the function $f(\xi)$ reflects the variation of the thermal diffusivity as a function of the coordinate, and $\varphi(\theta)$ reflects the variation of the rate of the chemical reaction as a function of the dimensionless temperature θ.

Scientific-Research Institute of Mathematics and Mechanics, Tomsk State University. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 38, No. 1, pp. 95-98, January, 1980. Original article submitted April 27, 1979.

0022-0841/80/3801-0066$07.50

TABLE 1. Comparison of the Exact Values of the Critical Parameters of a Thermal Explosion with the Approximate Values

n	δ_*, exact value	δ_*, calc. from (9)	θ_{0*}, exact value	θ_{0*}, calc. from (10)
0	0,88	0,865	1,2	1,17
1	2	2,02	1,386	1,36
2	3,32	3,49	1,6	1,55

$$\theta = \theta_0 (1 - \alpha\xi^2), \tag{5}$$

where

$$\alpha = \mathrm{Bi}/(\mathrm{Bi} + 2). \tag{6}$$

In (5) θ_0 is the maximum temperature at the center of the vessel, which depends on the intensity of the source.

We set up the necessary integral relation. To do this, making use of the symmetry condition (2), we write the heat flux at the point y in the form

$$y^n d\theta/dy = -\delta \int\limits_0^y \varphi(\theta)\,\xi^n d\xi. \tag{7}$$

The factor y^n takes account of the variation in the surface penetrated by the flux as y varies. Now we find the mean integral value of the heat flux† in the interval from 0 to 1 and, making use of the boundary condition (2) and also of formulas (4), (5), we find, after some simple calculations, that

$$\alpha\theta_0/\delta = (n+1)^{-1} + \gamma\beta_n\theta_0 + s_n\theta_0^2, \tag{8}$$

where

$$\beta_n = 0.5\,(n+1)^{-1} - \alpha\,(n+2)/[2\,(n+3)\,(n+4)],$$
$$s_n = 0.5\ (n+1)^{-1} - \alpha\,(n+2)/[(n+3)\,(n+4)] + \alpha^2\,(n+2)/[(2\,(n+5)\,(n+6)].$$

The critical conditions for the existence of real solutions for θ in (8) are the following:‡

$$\delta_* = \alpha/(\gamma\beta_n + \sqrt{2s_n/(n+1)}), \tag{9}$$

$$\theta_{0*} = 1/\sqrt{2s_n\,(n+1)}. \tag{10}$$

It should be noted that from (7) we can obtain other relations for δ_* and θ_{0*} (analogous to those given in [8]) if we set y = 1 in formula (7). The results obtained are less accurate and more sensitive to the choice of the approximate temperature profile.

We shall illustrate the accuracy of the results obtained in the most unfavorable case Bi → ∞, $\alpha \to 1$ (as Bi decreases, the accuracy of the calculation increases rapidly). The results for $\alpha = 1$, compared with the exact results of [1], are shown in Table 1. The error in the determination of δ_* does not exceed 5%.

2. Critical conditions for $f(\xi) \neq 1$. The solution of problem (1), (2), with $\varphi(\theta) = \mathrm{const}$, yields the following form of the trial profile:

$$\theta = \theta_0\,[1 - \alpha_1\psi(\xi)], \tag{11}$$

where

$$\psi(\xi) = \int\limits_0^\xi (x/f(x))\,dx, \quad \alpha_1 = \mathrm{Bi}/(1 + \mathrm{Bi}\,\psi(1)).$$

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†This method for averaging the heat flux is not the only one possible.

‡This determination of the critical conditions is equivalent to using the condition of strong parametric dependence $d\delta/d\theta_0 = 0$.

TABLE 2. Critical Values of δ_* for Different Values of A and Bi

A	Bi=10		Bi=100		Bi=1000	
	according to (12)	calculated (1)-(3)	according to (12)	calculated (1)-(3)	according to (12)	calculated (1)-(3)
20	3,98	4,26	7,59	6,92	8,51	8,49
50	5,37	5,25	11,22	10,96	15,85	14,45
80	5,62	5,89	14,12	13,49	22,39	20,41

After performing some simple calculations according to the above scheme, we obtain (setting n = 1)

$$\delta_* = \alpha_1/(3\gamma\Phi_1 + \sqrt{2\Phi_2}), \tag{12}$$

$$\theta_{0*} = 1/\sqrt{6\Phi_2}, \tag{13}$$

where

$$\Phi_1 = \int_0^1 dy \int_0^y \xi\,[1-\alpha_1\psi(\xi)]\,d\xi,$$

$$\Phi_2 = \int_0^1 dy \int_0^y \xi\,[1-\alpha_1\psi(\xi)]^2\,d\xi.$$

As an example, let us consider the critical conditions for ignition when a reactive gas flows in a turbulent regime through a long tube. The presence of a turbulent component of heat transfer makes the effective thermal diffusivity nonuniform. The simplest function $f(\xi)$ can be obtained by using Nikuradze's experiments [10]:

$$f(\xi) = 1 + A\xi(1-\xi),$$

where $A = 0.026\mathrm{Re}^{7/8}$.

The variation of $\delta_*(A)$ when Bi takes on different values is shown in Table 2. Formula (12) accurately reflects the qualitative property of attenuation of the function $\delta_*(A)$ as A increases, since as the turbulent transfer becomes more intensive, the effective temperature resistance of the reaction zone decreases, and the heat transfer is limited essentially by the thermal resistance of the wall.

There is good qualitative and quantitative agreement with the calculations of the initial problem (1)-(3) on computers, carried out in [11]. Attempts to use functions other than (1) as the trial functions (e.g., the parabola (5), for reasons of simplicity) lead not only to a loss of accuracy but also to an incorrect qualitative picture for large values of A.

Calculation of θ_* from (13), taking account of (14), indicates that $\theta_*(A)$ depends weakly on A (which is also confirmed by computer calculations performed in [11]). This justifies the use of the Gray–Harper approximation [9] and enables us to disregard in the ignition problem the effect of temperature pulsations on the heat-generation function (unlike the combustion regimes of [12]).

Thus, the method of integral relations can prove to be an effective method for finding the critical parameters of a thermal explosion in a system when the variability of the temperature field is essential. The limitations of the method lie largely in the possibility of representing the solution of the thermal problem for a constant source in a simple form. A conspicuous shortcoming of the method is that it is not clear whether the estimates obtained lie above or below the exact values.

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OCCURRENCE OF FREE CONVECTION IN A PLANE LAYER IN THE PRESENCE OF A CHEMICAL TRANSPORT REACTION

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UDC 536.25

We consider the conditions for the occurrence of natural convection when a volatile compound is transported through a gaseous phase as a result of a chemical reaction with a solid substance. We determine the variation of the critical Rayleigh number for the principal level of instability as a function of the parameters of the process.

In an infinite plane horizontal gaseous layer with solid boundaries we are given thermal boundary conditions of the first kind. On both of the boundaries there takes place a heterogeneous reversible exothermic reaction of the type $\nu_A A + \nu_S S \rightleftharpoons \nu_B B$; A is the initial gas; S, solid material of the wall; B, gaseous reaction product; ν_A, ν_S, ν_B, stoichiometric coefficients. The mixture of gases in the layer may be considered binary, since the reaction takes place in a heterogeneous manner and the vapor pressure of the solid material is negligibly small. For $T_1 > T_2$ (Fig. 1), since the reaction is exothermic, the thermodynamic equilibrium is shifted in such a way that the rate of the direct reaction, and consequently the gas flow rate A, on surface I will be less than on surface II. For the reaction product B the situation is reversed. The difference in concentrations gives rise to flows of the components caused by diffusion and convection. If the solid material of the surface takes part in the reaction, there will be mass Stefan flow in the system. In stationary conditions, the presence of Stefan flow is analogous to blowing into the system at a constant velocity. For the given conditions, there may be thermal and concentration nonuniformities in density in the mixture of gases. We write the concentration of the light component as $P_A/P = c$, and the density of the mixture as $\rho = \dfrac{P}{RT}[\mu_A + (\mu_A - \mu_B)c]$, μ_A, μ_B being the molecular masses of the components. Following [1], we shall assume that the density of the mixture admits of a linear expansion with respect to the average values of T and c, i.e., $\rho = \rho_0(1 - \beta_1 T' - \beta_2 c')$, where T' and c' are the deviations from the average values;

$$\beta_1 = -\frac{1}{\rho_0}\left(\frac{\partial\rho}{\partial T}\right)_{P,c}; \quad \beta_2 = -\frac{1}{\rho_0}\left(\frac{\partial\rho}{\partial c}\right)_{P,T}.$$

We write the equations of free convection of the mixture, considering it incompressible [1]. It should be noted that $\mathbf{v} = \mathbf{v}_c + \mathbf{v}_0$ is the total hydrodynamic velocity; $\mathbf{v}_c$ is the convective velocity; $\mathbf{v}_0$ is the Stefan velocity corresponding to the average density ρ_0.

Disregarding thermal diffusion and diffusive heat conduction in the heat and mass flows and assuming that the nonuniformity in density is essential only in the expression for the lifting force (the Boussinesq approximation), we obtain a system of equations,

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Institute of Chemical Physics, Moscow. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 38, No. 1, pp. 99-106, January, 1980. Original article submitted February 12, 1979.

0022-0841/80/3801-0069 \$07.50