SOLUTION OF A NONLINEAR PROBLEM IN HEAT CONDUCTIVITY INVESTIGATIONS

G. N. Gusenkov and I. M. Chirkov

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An approximate solution of the nonlinear heat conductivity equation is obtained using a method proposed earlier. This solution is convenient for use in the "ignition" criterion.

In the study of the processes of thermal decomposition of different materials and compounds by differential thermal analysis the problem of temperature distribution is of interest in the case when the specific heat and thermal conductivity of the sample change with the temperature and the very process of conversion is some source or sink of thermal energy. If T(x, t) is the temperature in the cell as a function of coordinate x and time t, α is the degree of conversion, E is the activation energy, and C(T), λ(T) are respectively the specific heat and the thermal conductivity of the investigated material or the solution, then the system of equations for the case, when the calorimetric cells have one of the classical forms, becomes

$$c_i(T_i)\frac{\partial T_i}{\partial t}=\frac{\partial}{\partial x}\left[\lambda_i(T_i)\frac{\partial T_i}{\partial x}\right]+\frac{k}{x}\lambda_i(T_i)\frac{\partial T_i}{\partial x}+H(i-1)\frac{d\alpha}{dt};\quad (1)$$

$$\frac{d\alpha}{dt}=\varphi(\alpha)A\exp\left(-\frac{E}{RT_2}\right);$$

$$T_i(x,\ 0)=T_0;\quad (2)$$

$$\lambda_i(T_i)\frac{\partial T_i}{\partial x}\bigg|_{x=\Delta}=q_i;\quad \frac{\partial T_i}{\partial x}\bigg|_{x=0}=0\quad (i=1,\ 2).\quad (3)$$

Here $\varphi(\alpha)$ is a function characterizing the order of reaction, H is the thermal effect of reaction (per unit volume), A is the preexponent, R is the gas constant, q is the intensity of the thermal flux which heats the cell containing the investigated material or the solution (i = 2) and the cell with the standard (i = 1), and Δ is the halfwidth of the layer of the material or the solution in the case of a plane cell (k = 0) and the radius in the case of the cylindical (k = 1) and spherical (k = 2) elements.

Here a characteristic feature is that very often the temperature dependence of c and λ can be assumed to be linear. In particular, this is always so when the initial temperature is not too different from the conversion temperature.

A similar problem is encountered in the physics of combustion of powders and explosive materials. It was here that a method of avoiding the difficulties associated with the need of solving a system of equations of type (1)-(3) was originally found. An "ignition" criterion was proposed [1], using which it was possible to restrict the investigation to the solution of partial differential equations in the analysis of a number of characteristics of the process. Apparently, this criterion can be used also in the case of thermal decomposition of other substances, since essentially these processes differ only in the amount of absorbed or liberated energy or in the order of reaction.

In the analysis of combustion processes the heat conductivity equation has been investigated under the assumption that c and λ are constant quantities. Even though this is not true in general, this approach gives reasonable results in the first approximation. In the study of the processes of thermal decomposition in conditions of scanning in a wide range of temperatures, this approximation is very rough. Therefore it is necessary to solve the nonlinear heat conductivity equation with nonlinear boundary conditions. Exact

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analytical solutions for this problem are not known for the general case. Below we present an approximate solution. This is done using the combined method proposed by us earlier [2].

Here we shall assume that the temperature at any point of theinvestigated sample can be represented in the form of a sum

$$T(x,\ t) = T(0,\ t) + \Delta T(x,\ t).$$

Here $\Delta T(x,\ t) \simeq \sqrt{\varepsilon} T(0,\ t)$ $(\varepsilon \ll 1)$, which is valid, for example, for small samples which are used in microcalorimetry. Besides, we shall assume that the slope of the straight lines $c(T)$, $\lambda(T)$ are also of the order of $\sqrt{\varepsilon}$.

Therefore, we write the heat conductivity equation with conditions (3) in dimensionless form:

$$\{1 + c_1\theta(0,\ \mathrm{Fo}) + \varepsilon\delta(\xi,\ \mathrm{Fo})\alpha\} \frac{\partial\theta}{\partial \mathrm{Fo}} = \frac{\partial}{\partial\xi}\left\{[1 + \lambda_1\theta(0,\ \mathrm{Fo}) + \varepsilon\delta(\xi,\ \mathrm{Fo})]\frac{\partial\theta}{\partial\xi}\right\}; \quad (4)$$

$$\{1 + \lambda_1\theta(0,\ \mathrm{Fo}) + \varepsilon\delta(\xi,\ \mathrm{Fo})\}\left.\frac{\partial\theta}{\partial\xi}\right|_{\xi=1} = \frac{q\Delta}{\lambda_0 T_0} = Q;$$

$$\left.\frac{\partial\theta}{\partial\xi}\right|_{\xi=0} = 0;\ \theta(\xi,\ 0) = 0; \quad (5)$$

Here

$$\theta = \frac{T - T_0}{T_0};\ \delta(\xi,\ \mathrm{Fo}) = \theta(\xi,\ \mathrm{Fo}) - \theta(0,\ \mathrm{Fo});\ \lambda = \lambda_0 + \lambda_{\sim}(T - T_0);$$

$$c = c_0 + c_{\sim}(T - T_0);\ c_1 = \frac{c_{\sim}}{c_0}T_0;\ \lambda_1 = \frac{\lambda_{\sim}}{\lambda_0}T_0;\quad \alpha = \frac{c_1}{\lambda_1};\ a_0 = \frac{\lambda_0}{c_0};$$

$$\frac{x}{\Delta} = \xi;\ \frac{a_0 t}{\Delta^2} = \mathrm{Fo}.$$

We shall seek the solution of systems (4), (5) in the form

$$\theta = f_1(\xi,\ \mathrm{Fo}) + \varepsilon f_2(\xi,\ \mathrm{Fo}) + \varepsilon^2 f_3(\xi,\ \mathrm{Fo}) + \cdots \quad (6)$$

We restrict ourselves to the first two terms in the expansion; then we have the following two equations for the functions f_1 and f_2:

$$[1 + c_1 f_1(0,\ \mathrm{Fo})]\frac{\partial f_1}{\partial \mathrm{Fo}} = [1 + \lambda_1 f_1(0,\ \mathrm{Fo})]\frac{\partial^2 f_1}{\partial\xi^2}; \quad (7)$$

$$[1 + c_1 f_1(0,\ \mathrm{Fo})]\frac{\partial f_2}{\partial \mathrm{Fo}} = [1 + \lambda_1 f_1(0,\ \mathrm{Fo})]\frac{\partial^2 f_2}{\partial\xi^2} + \left(\frac{\partial f_1}{\partial\xi}\right)^2$$
$$+ \left\{\lambda_1 f_2(0,\ \mathrm{Fo}) + f_1(\xi,\ \mathrm{Fo}) - f_1(0,\ \mathrm{Fo}) - [1 + \lambda_1 f_1(0,\ \mathrm{Fo})]\right.$$
$$\left.\times \frac{\alpha[f_1(\xi,\ \mathrm{Fo}) - f_1(0,\ \mathrm{Fo})] + c_1 f_2(0,\ \mathrm{Fo})}{1 + c_1 f_1(0,\ \mathrm{Fo})}\right\}\frac{\partial^2 f_1}{\partial\xi^2} \quad (8)$$
$$+ \frac{k[1 + \lambda_1 f_1(0,\ \mathrm{Fo})]}{\xi}\frac{\partial f_2}{\partial\xi} + \frac{k[\lambda_1 f_2(0,\ \mathrm{Fo}) + f_1(\xi,\ \mathrm{Fo}) - f_1(0,\ \mathrm{Fo})]}{\xi}\frac{\partial f_1}{\partial\xi}$$

with the boundary conditions for $f_1(\xi,\ \mathrm{Fo})$

$$[1 + \lambda_1 f_1(0,\ \mathrm{Fo})]\left.\frac{\partial f_1}{\partial\xi}\right|_{\xi=1} = Q;\quad \left.\frac{\partial f_1}{\partial\xi}\right|_{\xi=0} = 0; \quad (9)$$

and for $f_2(\xi,\ \mathrm{Fo})$

$$[1 + \lambda_1 f_1(0,\ \mathrm{Fo})]\frac{\partial f_2}{\partial\xi} + \lambda_1 f_2(0,\ \mathrm{Fo})\left.\frac{\partial f_1}{\partial\xi}\right|_{\xi=1} = 0;$$
$$\left.\frac{\partial f_2}{\partial\xi}\right|_{\xi=0} = 0;\ f_1(\xi,\ 0) = f_2(\xi,\ 0) = 0. \quad (10)$$

Let us find the main part in expansion of θ. According to [2] we express $f_1(\xi,\ \mathrm{Fo})$ in the form

$$f_1(\xi,\ \mathrm{Fo}) = f_{11}(\xi,\ \mathrm{Fo}) + f_{12}(\xi,\ \mathrm{Fo}). \quad (11)$$

Since $f_{11}(\xi, \text{Fo})$ must satisfy conditions (9) and $f_{12}(\xi, \text{Fo})$ must satisfy the homogeneous conditions we have

$$f_1(\xi, \text{Fo}) = a + \frac{Q\xi^2}{2(1+\lambda_1 a)} + b(\xi^4 - 2\xi^2), \tag{12}$$

where $a(\text{Fo})$ must be determined from Eq. (7) after substituting f_{11} into it and integrating over ξ in the limits from 0 to 1, and $b(\text{Fo})$ must be found from Galerkin condition, in which the function $X(\xi) = \xi^4 - 2\xi^2$ should be used as the moment. Thus for $a(\text{Fo})$ and $b(\text{Fo})$ we obtain

$$\frac{da}{d\text{Fo}} = \frac{Q}{(1+c_1 a)\left[\dfrac{1}{k+1} - \dfrac{Q\lambda_1}{2(k+3)(1+\lambda_1 a)^2}\right]}; \tag{13}$$

$$\frac{db}{da} + f(a)\, b = g(a);$$

$$f(a) = \frac{128(1+\lambda_1 a)\left[\dfrac{1}{k+1} - \dfrac{Q\lambda_1}{2(k+3)(1+\lambda_1 a)^2}\right]}{(k+3)(k+5)(k+7)Q\left[\dfrac{1}{k+9} + \dfrac{4}{k+5} - \dfrac{4}{k+7}\right]}; \tag{14}$$

$$G(a) = -\frac{16Q\lambda_1}{(k+3)^2(k+5)(k+7)(1+\lambda_1 a)^2\left[\dfrac{1}{k+9} + \dfrac{4}{k+5} - \dfrac{4}{k+7}\right]}.$$

Equations (13), (14) may be solved in quadratures. However, the formulas obtained in this way are complicated. Therefore, for simplification we shall make use of the following fact. Remembering that λ_1 and c_1 are of the order of $\sqrt{\varepsilon}$ the implicit expression for $a(\text{Fo})$, obtained after integration of Eq. (13), and the coefficients of Eq. (14) can be represented in the form of power series of $\sqrt{\varepsilon}$. Since from the very beginning we have restricted ourselves to two terms in expansion (6), in determining $a(\text{Fo})$ it is sufficient to keep the same accuracy, i.e., to retain only up to quadratic terms. Remembering that the combined method gives a small correction at the second stage, in the determination of $b(\text{Fo})$ it is sufficient to retain only terms not including the products $\lambda_1 a$ or $\lambda_1 c$.

Thus we obtain

$$a = [-[2(k+3) - Q\lambda_1(k+1)] + \{[2(k+3) - Q\lambda_1(k+1)]^2$$
$$+ 4(k+1)(k+3)Q\,\text{Fo}\,[2(k+3)c_1 - Q\lambda_1(k+1)(2\lambda_1+c_1)]\}^{0.5}]\,[2(k+3)c_1 - Q\lambda_1(k+1)(2\lambda_1+c_1)]^{-1}; \tag{15}$$

$$b = -\frac{Q^2\lambda_1}{8(k+3)\left[\dfrac{1}{k+1} - \dfrac{Q\lambda_1}{2(k+3)}\right]}$$
$$\times\left\{1 - \exp\left[\frac{128a\left(\dfrac{Q\lambda_1}{2(k+3)} - \dfrac{1}{k+1}\right)}{(k+3)(k+5)(k+7)Q}\,\frac{1}{\left(\dfrac{1}{k+9} + \dfrac{4}{k+5} - \dfrac{4}{k+7}\right)}\right]\right\}. \tag{16}$$

Let us now find $f_2(\xi, \text{Fo})$. Here we shall restrict ourselves only to the solution obtained by the integral method, since as already mentioned, the correction associated with the use of combined method will be of the order of the term after εf_2 in (6).

Representing f_2 in the form

$$f_2(\xi, \text{Fo}) = \alpha_0(\text{Fo}) + \alpha_1(\text{Fo})\,\xi + \alpha_2(\text{Fo})\,\xi^2$$

and considering boundary conditions (10), according to the integral method we have

$$f_2 = \alpha_0\left\{1 - \frac{\lambda_1 Q\xi^2}{2(1+\lambda_1 a)^2}\right\} + \frac{Q - 2b(1+\lambda_1 a)}{4(1+\lambda_1 a)^3}\,Q\xi^2. \tag{17}$$

After averaging (8) over ξ for $\alpha_0(\text{Fo})$ we obtain a linear differential equation with variable coefficients. For the sake of simplicity we write the integral of this equation in the approximation used above, i.e., neglecting terms of order of $\sqrt{\varepsilon}$ and higher compared to unity. As a result we have

$$\alpha_0 = \frac{Q(k+1)}{2c_1}\left(2 + \frac{\alpha}{k+3}\right)\{1 - \exp[-Qc_1\text{Fo}]\}. \tag{18}$$

Formula (6), (12), (17) give the solution of the problem with an accuracy up to terms with $\varepsilon^{3/2}$. Here a characteristic feature is that in these formulas the dependence on the coordinate is represented by a biquadratic polynomial. If we consider that in the vicinity of the conversion temperature the function exp(—E /RT) in the "ignition" criterion [1] can be expanded in power series of T^{-k} (k = 0, 1, 2, ...), this form of the solution is very convenient for further computations.

NOTATION

T	is the temperature;
x	is the coordinate;
t	is the time;
α	is the degree of conversion;
E	is the activation energy;
C	is the specific heat;
λ	is the thermal conductivity;
$\varphi(\alpha)$	is a function characterizing the order of reaction;
H	is the thermal effect of reaction;
A	is the preexponant;
K	is the gas constant;
q_i	is the intensity of the heat flux delivered to the cells with the investigative material (i = 2) and standard (i = 1);
Δ	is the halfwidth of the layer of the material;
θ, Q, ξ	are the temperature, heat flux, and coordinate;
Fo	is the Fourier number.

LITERATURE CITED

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