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# PARAMETRIC ANALYSIS OF SITE MODES OF THERMAL EXPLOSIONS BY A "GEOMETRICAL-OPTICAL" ASYMPTOTIC METHOD

**A. V. Kotovich and G. A. Nesenenko** UDC 541.124

*Asymptotic formulas describing the modes of site thermal explosions with an arbitrary initial distribution of temperature and results of calculation by these formulas are presented. A comparison with the data obtained by other authors is made and the effect of the presence of two "traveling waves" is revealed.*

Practical interest in the processes of thermal explosion is associated mainly with problems of safety in certain kinds of work with explosives – treatment, production, carrying out of blastings in high-temperature wells, etc. In many cases, on the basis of thermal-explosion theory, it is possible, in principle, to precalculate safe conditions which eliminate spontaneous origination of explosion.

By virtue of the importance of the site modes of a thermal explosion, different authors studied them using numerical experiments and approximate analytical methods, in particular, asymptotic ones [1-4]. We note that the significance of asymptotic methods increases if the initial distribution of temperature in a substance is arbitrary [3], since in this case a parametric analysis of the modes of a site thermal explosion is possible [4].

This work briefly describes the results of a parametric analysis of the modes of a site thermal explosion. It is based on the use of a mathematically correct "geometrical-optical" asymptotic method [5].

A mathematical formulation of the problem of a site thermal explosion (without regard for the burnout of a substance – a zeroth-order reaction) in dimensionless parameters suggested by Frank-Kamenetskii has the form [1-4]

$$\frac{\partial \Theta}{\partial \tau} = \varepsilon \frac{\partial^2 \Theta}{\partial \xi^2} + \beta \exp\left\{\frac{\Theta}{1 + \mathrm{Ar}\,\Theta}\right\}; \tag{1}$$

$$\Theta(\xi, \tau) = \Theta^0(\xi), \quad \tau = +0, \quad -\infty < \xi < \infty; \tag{2}$$

$$\frac{\partial \Theta(\xi, \tau)}{\partial \xi} \to 0, \quad \xi \to \pm\infty, \tag{3}$$

where $\varepsilon = \mathrm{Fk}^{-1}$ and $\beta$ is introduced for the convenience of further presentation: $\beta$ is equal either to zero – then the function $\Theta(\xi, \tau)$ describes a solution of the "inert" Cauchy problem, or to unity – then the function $\Theta(\xi, \tau)$ describes a site thermal explosion. The smallness of the parameter $\varepsilon = \mathrm{Fk}^{-1}$ is a special property of the modes of a site thermal explosion in condensed media [1-3]. This allows one to write the solution $\Theta(\xi, \tau)$ of the Cauchy problem in the form [4]

$$\Theta(\xi, \tau) \underset{\varepsilon \to 0}{\sim} d_0(\xi, \tau) + \varepsilon d_1(\xi, \tau) + \varepsilon^2 d_2(\xi, \tau) + \dots, \tag{4}$$

where, by virtue of the small values of the Arrhenius number [1, 2], the coefficients $d_i(\xi, \tau)$ can in turn be represented as [4]

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$$d_i(\xi,\tau) = d_i^{(0)}(\xi,\tau) + \mathrm{Ar}\, d_i^{(1)}(\xi,\tau) + \mathrm{Ar}^2 d_i^{(2)}(\xi,\tau) + \ldots \tag{5}$$

For example,

$$d_0^{(0)}(\xi,\tau) = -\ln\left[\exp(-\Theta^0(\xi)) - \beta\tau\right], \tag{6}$$

$$d_0^{(1)}(\xi,\tau) = (\ln\left[\exp(-\Theta^0(\xi)) - \beta\tau\right] - 1)^2 + 1 - \frac{B\exp(-\Theta^0(\xi))}{\exp(-\Theta^0(\xi)) - \beta\tau}, \tag{7}$$

$$\begin{aligned} d_0^{(2)}(\xi,\tau) = &- \ln^3\left[\exp(-\Theta^0(\xi)) - \beta\tau\right] + 5\ln^2\left[\exp(-\Theta^0(\xi)) - \beta\tau\right] - \\ &- 10\ln\left[\exp(-\Theta^0(\xi)) - \beta\tau\right] + 10 - \frac{4\beta\tau}{\exp(-\Theta^0(\xi)) - \beta\tau} - \\ &- \frac{4B\exp(-\Theta^0(\xi))\ln\left[\exp(-\Theta^0(\xi)) - \beta\tau\right]}{\exp(-\Theta^0(\xi)) - \beta\tau} - \frac{B^2\exp(-2\Theta^0(\xi))}{\left[\exp(-\Theta^0(\xi)) - \beta\tau\right]^2} + \\ &+ \frac{\left\{-[\Theta^0(\xi)]^3 - 5[\Theta^0(\xi)]^2 - 10\Theta^0(\xi) - 10 - 4B\Theta^0(\xi) + B^2\right\}\exp(-\Theta^0(\xi))}{\exp(-\Theta^0(\xi)) - \beta\tau}, \end{aligned} \tag{8}$$

$$\begin{aligned} d_1^{(0)}(\xi,\tau) = &\frac{1}{\exp(-\Theta^0(\xi)) - \beta\tau} \times \\ &\times \left\{ \tau\exp(-\Theta^0(\xi))\left\{(\Theta^0(\xi))^3 - [(\Theta^0(\xi))']^2\right\} - \frac{\Theta^0(\xi)\,[(\Theta^0(\xi))']^2}{\beta}\exp\left\{-2\Theta^0(\xi)\right\} - \right. \\ &\left. - \frac{[(\Theta^0(\xi))']^2\exp(-2\Theta^0(\xi))}{\beta}\ln\left[\exp(-\Theta^0(\xi)) - \beta\tau\right] \right\}, \end{aligned} \tag{9}$$

where $B = 1 + [\Theta^0(\xi) + 1]^2$.

The details of deriving formulas (4)-(9) can be found in [4], where a rather thorough analytical comparison of the asymptotics in terms of the Poincaré (4) solution $\Theta(\xi, \tau)$ with the results obtained by other authors is made.

In the present work, the authors studied the effect of such parameters as: 1) the Arrhenius number, 2) the Frank-Kamenetskii criterion (by varying a small dimensionless parameter $\varepsilon = \mathrm{Fk}^{-1}$), 3) the degree of influence of evaluated terms of the asymptotics in formulas (5) on the mode of a site thermal explosion described by the solution $\Theta(\xi, \tau)$ of the Cauchy problem (1)-(3). We note that this parametric analysis of the processes of thermal ignition of condensed media, which uses asymptotic formulas obtained by a "geometrical-optical" asymptotic method, was made in [6].

The initial distribution $\Theta^0(\xi)$ of the dimensionless heating $\Theta(\xi, \tau)$ was assumed to be Gaussian, which, in the dimensionless system of coordinates used, corresponds to an analytical expression

$$\Theta^0(\xi) = \Theta(\xi,\tau)\big|_{\tau=0} = \frac{[T_{\mathrm{in}}(\xi r) - T_0]\,E}{RT_0^2}, \tag{10}$$

where $T_{\mathrm{in}}(x) = \exp\{-x^2\}$.

TABLE 1. Dimensionless Time $\tau$ as a Function of Dimensionless Heating $\Theta = d_0 = d_0^{(0)} + \mathrm{Ar} d_0^{(1)} + \mathrm{Ar}^2 d_0^{(2)}$ at $\varepsilon = 0$, $\Theta^0 = 0$, $T_0 = 1$ and Various Arrhenius Numbers Ar

| Ar | $\tau$ | 0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.55 | 0.6 | 0.65 | 0.7 | 0.75 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.03 | $\Theta$ | 0 | 0.105 | 0.223 | 0.356 | 0.509 | 0.688 | 0.79 | 0.903 | 1.029 | 1.17 | 1.33 |
| 0.01 | $\Theta$ | 0 | 0.105 | 0.223 | 0.356 | 0.51 | 0.692 | 0.796 | 0.913 | 1.044 | 1.195 | 1.371 |
| 0.001 | $\Theta$ | 0 | 0.105 | 0.223 | 0.357 | 0.511 | 0.693 | 0.798 | 0.916 | 1.049 | 1.203 | 1.385 |
| Ar | $\tau$ | 0.8 | 0.85 | 0.859 | 0.9 | 0.904 | 0.944 | 0.95 | 0.964 | 0.99 | 0.994 | 0.996 |
| 0.03 | $\Theta$ | 1.509 | 1.702 | 1.736 | 1.844 | 1.845 | | | | | | |
| 0.01 | $\Theta$ | 1.584 | 1.849 | 1.903 | 2.198 | 2.23 | 2.59 | 2.645 | 2.717 | | | |
| 0.001 | $\Theta$ | 1.607 | 1.893 | 1.954 | 2.294 | 2.334 | 2.862 | 2.971 | 3.286 | 4.401 | 4.715 | 4.824 |

TABLE 2. Dimensionless Time $\tau$ as a Function of Dimensionless Heating $\Theta$ Obtained by the Todes Formula at $\varepsilon = 0$, $\beta = 1$, $\xi = 0$, $\Theta^0 = 0$ and Various Arrhenius Numbers Ar

| Ar | $\tau$ | 0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.55 | 0.6 | 0.65 | 0.7 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.03 | $\Theta$ | 0 | 0.105 | 0.223 | 0.356 | 0.509 | 0.689 | 0.702 | 0.907 | 1.035 | 1.181 |
| 0.01 | $\Theta$ | 0 | 0.105 | 0.223 | 0.356 | 0.51 | 0.692 | 0.796 | 0.913 | 1.045 | 1.196 |
| 0.001 | $\Theta$ | 0 | 0.105 | 0.223 | 0.357 | 0.511 | 0.693 | 0.798 | 0.916 | 1.049 | 1.203 |
| Ar | $\tau$ | 0.75 | 0.8 | 0.85 | 0.859 | 0.9 | 0.944 | 0.95 | 0.99 | 0.994 | |
| 0.03 | $\Theta$ | 1.35 | 1.551 | 1.796 | 1.847 | | | | | | |
| 0.01 | $\Theta$ | 1.374 | 1.588 | 1.86 | 1.917 | 2.229 | 2.715 | | | | |
| 0.001 | $\Theta$ | 1.385 | 1.607 | 1.893 | 1.955 | 2.295 | 2.863 | 2.973 | 4.453 | 4.862 | |

We begin a parametric analysis of properties of the solution $\Theta(\xi, \tau)$ of the boundary-value problem (1)-(3) from the case where $\varepsilon = 0$, since here

$$\Theta(\xi, \tau) \underset{\varepsilon \to 0}{\sim} d_0(\xi, \tau) . \tag{11}$$

For Ar << 1, the asymptotics of the function $d_0(\xi\ \tau)$ has the form

$$d_0(\xi, \tau) = d_0^{(0)}(\xi, \tau) + \mathrm{Ar}\, d_0^{(1)}(\xi, \tau) + \mathrm{Ar}^2 d_0^{(2)}(\xi, \tau) + O(\mathrm{Ar}^3) , \tag{12}$$

where the coefficients $d_0^{(0)}(\xi, \tau)$, $d_0^{(1)}(\xi, \tau)$, and $d_0^{(2)}(\xi, \tau)$ are assigned by analytical expressions (6)-(8), respectively. The function $d_0(\xi, \tau)$ is a solution of the Cauchy problem

$$\frac{\partial d_0}{\partial \tau} = \beta \exp\left\{\frac{d_0}{1 + \mathrm{Ar}\, d_0}\right\} , \tag{13}$$

$$d_0(\xi, \tau) \to \Theta^0(\xi) , \quad \tau \to +0 , \tag{14}$$

and the solution $d_0(\xi, \tau)$ of the Cauchy problem (13) and (14) was studied earlier by other authors within the framework of the model of "adiabatic thermal explosion" [2].

Graphs of the solution $d_0(\xi, \tau)$ obtained as a result of numerical calculations on a computer are given in [2]. It follows from them that the solution $d_0(\xi, \tau)$ of the Cauchy problem (13), (14) is a limited function monotonically increasing with time.

An analytical solution of the Cauchy problem (13), (14) was obtained by Todes (the "Todes solution" [2]) and has the following form (the notation adopted in the present paper is used):

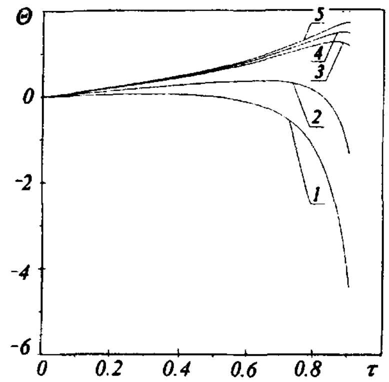


Fig. 1. Dimensionless heating $\Theta = d_0 + \varepsilon d_1^{(0)}$ vs. dimensionless time $\tau$ at Ar = 0.03, $\beta = 1$, $\xi = 0$, $\varepsilon = 0.001$ (1), $\varepsilon = 0.005$ (2), $\varepsilon = 0.001$ (3), $\varepsilon = 0.0005$ (4), and $\varepsilon = 0.0001$ (5).

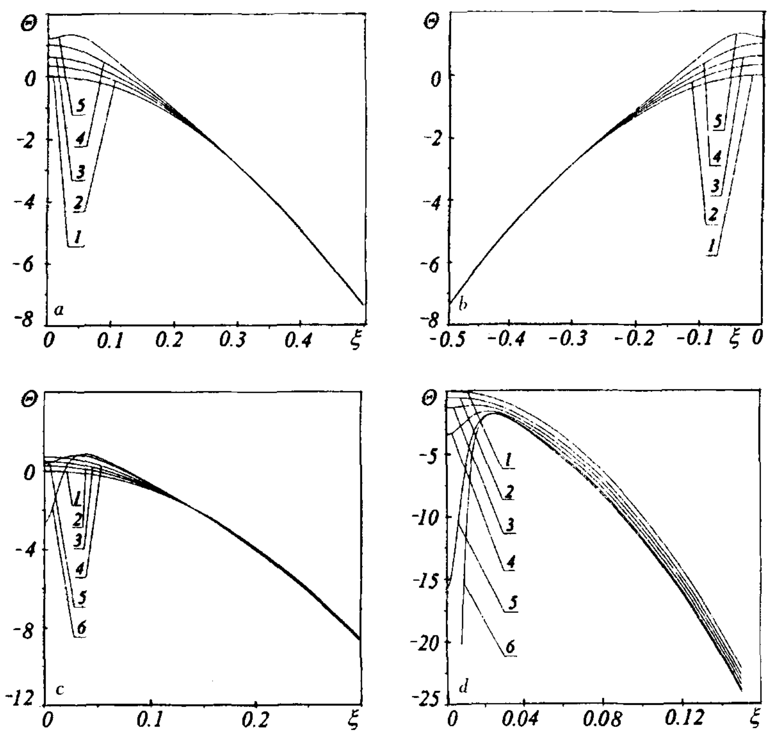


Fig. 2. Dimensionless heating $\Theta = d_0 + \varepsilon d_1^{(0)}$ vs. dimensionless coordinate $\xi$ at $\varepsilon = 0.001$, $\beta = 1$: a, b) 1) $\tau = 0$; 2) 0.3; 3) 0.5; 4) 0.7; 5) 0.904 (Ar = 0.03); c) 1-4) see a, b); 5) $\tau = 0.9$; 6) 0.964 (Ar = 0.01); d) 1-4) see a, b); 5) $\tau = 0.9$; 6) 0.996 (Ar = 0.001).

$$\tau \underset{\mathrm{Ar}\to 0}{\simeq} \frac{\exp\left\{-\frac{1}{\mathrm{Ar}}\right\}}{\mathrm{Ar}} \left[ (1 + \mathrm{Ar}\,\Theta^0) \exp\left\{\frac{1}{\mathrm{Ar}\,(1 + \mathrm{Ar}\,\Theta^0)}\right\} \times \right.$$

$$\left. \times \sum_{k=1}^{\infty} k\,!\,\mathrm{Ar}^k (1 + \mathrm{Ar}\,\Theta^0)^k - (1 + \mathrm{Ar}\,\Theta) \exp\left\{\frac{1}{\mathrm{Ar}\,(1 + \mathrm{Ar}\,\Theta)}\right\} \sum_{k=1}^{\infty} k\,!\,\mathrm{Ar}^k (1 + \mathrm{Ar}\,\Theta)^k \right]. \qquad (15)$$

To show the accuracy of the obtained asymptotic formula (12), the authors made comparative calculations by formula (12) (see Table 1) and by the "Todes formula" (15) (see Table 2). The data presented show good agreement of the results and indicate that allowance for the terms of the asymptotics (Ar << 1) in formula (12) exerts a considerable effect on the accuracy of calculation of $\tau = \tau(\Theta)$. The divergence in values of $\tau$ in Table 1 and Table 2 is explained by the fact that at Ar = 0.03 a small number of terms is allowed for in formula (12), i.e., if terms of the order of $O(\mathrm{Ar}^3)$ are taken into account, then Tables 1 and 2 will agree more completely.

Figure 1 presents the values of $\Theta = \Theta(\tau)$ at $\xi = 0$ as functions of different values of $\varepsilon = \mathrm{Fk}^{-1}$. The figure shows complete qualitative agreement with the results obtained in [1].

Of greatest interest to the authors are the data of parametric analysis of a site thermal explosion given in Fig. 2. It follows from these graphs that, first, the curves $\Theta = \Theta(\xi)$ are even functions and, second, the initial "Gaussian" distribution (10), which is symmetric at the initial instant of time $\tau = 0$, forms, as time goes, two "traveling waves," one of which moves toward $\xi = +\infty$ and the other toward $\xi = -\infty$. In this case, the amplitude of these "traveling waves" decreases with decrease in Ar.

It is of interest to note that in many works describing a solution of nonstationary problems of heat conduction with nonlinear heat sources the presence of "traveling-wave" solutions is indicated [2, 7]. Nevertheless, R. S. Burkina and coauthors [3], who studied the modes of site thermal explosions with variable initial conditions, failed to record the effect shown in Fig. 2.

The asymptotic relations (4)-(9) given above can be refined by addition of terms (with respect to $\varepsilon$ and Ar) so that they can be used for more thorough parametric analysis of the modes of a site thermal explosion [1].

## NOTATION

$\Theta = (T - T_0)E/RT_0^2$, heating of the substance; $\xi = x/r$, spatial coordinate; $\tau = t/t^*$, time; $r$ and $t^* = (c\rho RT_0^2)/(QEk(T_0))$, adiabatic scale of time; $T = T(x, t)$, temperature in the zone of reaction; $T_0$, ambient temperature; $R$, gas constant; $E$, activation energy; $c$, heat capacity; $\rho$, density; $\mathrm{Ar} = RT_0/E$, Arrhenius number; $\mathrm{Fk} = QEr^2k(T_0)/(\lambda RT_0^2)$, Frank-Kamenetskii criterion; $Q$, heat effect of the reaction (per unit volume); $k(T)$, characteristic rate constant of the reaction at temperature $T$: $k(T) = K_0 \exp\{-E/RT\}$; $K_0$, preexponential factor; $T_{\mathrm{in}}(x)$, distribution of temperature at the initial instant of time.

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