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Behavior of the Temperature and Burnup of a Reactive Body at the Surface $x = 0$ upon Thermal Ignition

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Using the Laplace transform, we show that equations that govern the evolution with time of the temperature and burnup of a reactive body in the cross section $x = 0$ in the processes of thermal ignition can be derived. The equations for the temperature and burnup of a semibounded body at the ignition point $x = 0$ are obtained when the ignition is initiated by a radiation flux and in the case of thermal explosion of a hot spot. An asymptotic analysis of the equations obtained is carried out, and the ignition times of bodies and the critical conditions for ignition of a hot spot are determined. Vilyunov's "adiabatic method" of obtaining the temporal ignition characteristics is justified. The results of the asymptotic analysis of the ignition of a hot-spot are supported.

In the induction regimes of the thermal theory of ignition, the criterion of ignition and the ignition time of a system are determined by the behavior of the temperature at the ignition point. The main problem for these processes is to find the ignition point and the law of temperature variation at this point. For ignition of bodies with a monotonically increasing surface temperature (e.g., in the case of ignition by a radiant heat flux), Vilyunov proposed an "adiabatic method of ignition" [1, 2], in which, to obtain the temperature of the ignition surface, the total period of ignition is divided into the stage of inert heating and the adiabatic stage of chemical reactions near the body surface; the "matching" of these stages allows one to determine the general law of change of the surface temperature and the temporal characteristics of ignition. The splitting of the process into the stages is due to the large ratio between the heating time and the time of adiabatic chemical reactions [2]. Kim and Chung [3, 4] studied the ignition of porous combustible materials by a heat flux in the case where a gaseous oxidant diffuses through their external boundaries from the ambient medium. For large activation energies and the Lewis number $\mathrm{Le} = 1$, they used the Laplace integral transform and the method of asymptotic integration to obtain an ordinary differential equation for the temperature of the body surface. The numerical solution of this equation made it possible to obtain information on the ignition and its parameters. The applicability of the Laplace and Hankel integral transforms to obtaining of the heating characteristics of a body during inert heating of this body by a radiation flux with a space-distributed density was shown by Gusachenko [5]. The resulting expressions for the temperature and its derivatives in the region of maximum heating were then used for calculating the ignition time of the reactive body.

In the present paper, we study the possibility of deriving differential equations for the temperature and the burnup at the ignition point $x = 0$ by referring to two problems: ignition of nontransparent and semitransparent reactive bodies by a radiation flux and ignition of a hot spot. Subsequent asymptotic analysis of these equations for large values of the temperature drop $\Theta_0 \gg 1$ allows us to obtain desired information on the ignition process. In particular, the results of this investigation for the problem of ignition by a heat flux validate Vilyunov's adiabatic method.

We first consider the problem of ignition of a semibounded reactive body by a radiant heat flux incident upon the body surface $x = 0$. In dimensionless variables, the mathematical formulation of the problem has the form

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} - B\exp(-B\xi)$$

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$$- \omega(1-\eta)^m \exp\Big(-\frac{\Theta_0 u}{1-\sigma u}\Big); \quad (1)$$

$$\frac{\partial \eta}{\partial \tau} = \mathrm{Le}\frac{\partial^2 \eta}{\partial \xi^2} + \gamma\omega(1-\eta)^m \exp\Big(-\frac{\Theta_0 u}{1-\sigma u}\Big), \quad (2)$$

$$\tau > 0, \quad 0 < \xi < \infty;$$

$$u(\xi, 0) = 1, \quad \eta(\xi, 0) = 0; \quad (3)$$

$$\frac{\partial \eta(0,\tau)}{\partial \xi} = \frac{\partial u(\infty,\tau)}{\partial \xi} = \frac{\partial \eta(\infty,\tau)}{\partial \xi} = 0; \quad (4)$$

$$\frac{\partial u(0,\tau)}{\partial \xi} = \begin{cases} 0, & B \neq \infty, \\ 1, & B = \infty. \end{cases} \quad (5)$$

In (1)–(5), the following dimensionless variables and parameters were used:

$$u = \frac{T_* - T}{T_* - T_0}, \quad \eta = \frac{a_0 - a}{a_0}, \quad \xi = \frac{x}{x_\mathrm{h}},$$

$$\tau = \frac{t}{t_\mathrm{h}}, \quad x_\mathrm{h} = \lambda\frac{T_* - T_0}{q}, \quad t_\mathrm{h} = \frac{c\rho x_\mathrm{h}^2}{\lambda},$$

$$B = n x_\mathrm{h}, \quad \Theta_0 = E\frac{T_* - T_0}{RT_*^2},$$

$$\omega = \frac{Q z \rho^m a_0^m \lambda (T_* - T_0)\exp(-E/RT_*)}{q^2},$$

$$\sigma = \frac{T_* - T_0}{T_*}, \quad \mathrm{Le} = \frac{c\rho D}{\lambda}, \quad \gamma = c\frac{T_* - T_0}{Q a_0}.$$

The notation is as follows: T and T_* are the current and scaling temperatures (the latter one is not yet defined), T_0 is the initial temperature of the combustible component, x is the spatial coordinate, t is the time, τ is the dimensionless time variable, a and a_0 are the current and initial concentrations of the reacting substance, q is the density of the external radiation flux, x_h and t_h are the spatial and temporal characteristic scales for the inert-heating stage, c is the specific heat, ρ is the density, λ is the thermal conductivity, n is the absorption coefficient of the radiant heat flux, Q is the heat of the chemical reaction, E is the activation energy, R is the gas constant, z is the preexponent, D is the diffusion coefficient, m is the order of the chemical reaction, u is the temperature in the variables of heating, η is the burnup, and ξ and τ are the spatial and temporal variables.

For subsequent analysis, we pass from the dimensionless temperature u to a variable that characterizes heating of the system by chemical reactions: $\varphi = u - u_I$, where $u_I(\xi, \tau)$ is the solution of the problem of inert heating of a body by an external radiation flux:

$$\frac{\partial u_I}{\partial \tau} = \frac{\partial^2 u_I}{\partial \xi^2} - B\exp(-B\xi), \quad (6)$$

$$\tau > 0, \quad 0 < \xi < \infty;$$

$$u_I(\xi, 0) = 1, \quad \frac{\partial u_I(\infty,\tau)}{\partial \xi} = 0, \quad (7)$$

$$\frac{\partial u_I(0,\tau)}{\partial \xi} = \begin{cases} 0, & B \neq \infty, \\ 1, & B = \infty. \end{cases}$$

Then, problem (1)–(5) takes the form

$$\frac{\partial \varphi}{\partial \tau} = \frac{\partial^2 \varphi}{\partial \xi^2} - \omega(1-\eta)^m \times \exp\Big[-\frac{\Theta_0(\varphi + u_I)}{1 - \sigma(\varphi + u_I)}\Big]; \quad (8)$$

$$\frac{\partial \eta}{\partial \tau} = \mathrm{Le}\frac{\partial^2 \eta}{\partial \xi^2}\gamma\omega(1-\eta)^m \times \exp\Big[-\frac{\Theta_0(\varphi + u_I)}{1 - \sigma(\varphi + u_I)}\Big], \quad (9)$$

$$\tau > 0, \quad 0 < \xi < \infty;$$

$$\varphi(\xi, 0) = \eta(\xi, 0) = 0; \quad (10)$$

$$\frac{\partial \varphi(0,\tau)}{\partial \xi} = \frac{\partial \eta(0,\tau)}{\partial \xi} = 0, \quad \frac{\partial \varphi(\infty,\tau)}{\partial \xi} = \frac{\partial \eta(\infty,\tau)}{\partial \xi} = 0. \quad (11)$$

We apply the Laplace integral transform to problem (8)–(11) and pass to the Laplace transform in the spatial variable

$$\xi \to S, \quad \varphi(\xi,\tau)\text{–}\bar{\varphi}(S,\tau), \quad \eta(\xi,\tau)\text{–}\bar{\eta}(S,\tau).$$

Then, from (8)–(11), we have

$$\frac{d\bar{\varphi}}{d\tau} = S^2\bar{\varphi}(S,\tau) - S\varphi(0,\tau) - J(S,\tau), \quad (12)$$

$$\frac{d\bar{\eta}}{d\tau} = \mathrm{Le}[S^2\bar{\eta}(S,\tau) - S\eta(0,\tau)] + \gamma J(S,\tau), \quad (13)$$

$$\bar{\varphi}(S,0) = \bar{\eta}(S,0) = 0, \quad (14)$$

where

$$J(S,\tau) = \int_0^\infty \omega[1-\eta(\xi,\tau)]^m \times \exp\Big[-\frac{\Theta_0(\varphi(\xi,\tau) + u_I(\xi,\tau))}{1 - \sigma(\varphi(\xi,\tau) + u_I(\xi,\tau))}\Big]\exp(-S\xi)d\xi$$

is the Laplace transform of the inhomogeneous parts in Eqs. (8) and (9). Integration of the ordinary differential equations (12)–(14) over the variable τ yields

$$S\bar{\varphi}(S,\tau) = \varphi(0,\tau) - \int_0^\tau \Big[\frac{\partial\varphi(0,y)}{\partial y} + SJ(S,y)\Big] \times \exp[(\tau - y)S^2]dy, \quad (15)$$

$$S\bar{\eta}(S,\tau) = \eta(0,\tau) - \int_0^\tau \Big[\frac{\partial\eta(0,y)}{\partial y} - \gamma SJ(S,y)\Big] \times \exp[(\tau - y)\mathrm{Le}S^2]dy. \quad (16)$$

Passing in (15) and (16) to the limit as $S \to \infty$ and taking into account that, for the Laplace transform, the limiting relation

$$\lim_{S\to\infty} S\bar{f}(S,\tau) = f(0,\tau)$$

holds, we obtain the following equations for the heating and burnup at the body surface $\xi = 0$:

$$\frac{\partial\varphi(0,\tau)}{\partial\tau} + \omega[1-\eta(0,\tau)]^m \times \exp\Big[-\frac{\Theta_0(\varphi(0,\tau)+u_I(0,\tau))}{1-\sigma(\varphi(0,\tau)+u_I(0,\tau))}\Big] = 0, \quad (17)$$

$$\frac{\partial\eta(0,\tau)}{\partial\tau} - \gamma\omega[1-\eta(0,\tau)]^m \times \exp\Big[-\frac{\Theta_0(\varphi(0,\tau)+u_I(0,\tau))}{1-\sigma(\varphi(0,\tau)+u_I(0,\tau))}\Big] = 0, \quad (18)$$

$$\varphi(0,0) = \eta(0,0) = 0. \quad (19)$$

System (17)–(19) has the first integral

$$\eta(0,\tau) = -\gamma\varphi(0,\tau), \quad (20)$$

which shows the similarity between the heating by chemical reactions and the burnup at the body surface for any value of the parameter Le. In what follows, we denote the values of the variables at the surface $\xi = 0$ by the subscript s: $\varphi(0,\tau) = \varphi_s(\tau)$. Substitution of the integral (20) into Eq. (17) yields an independent problem for heating by chemical reactions at the body surface:

$$\frac{d\varphi_s(\tau)}{d\tau} + \omega[1+\gamma\varphi_s(\tau)]^m \times \exp\Big[-\frac{\Theta_0(\varphi_s(\tau)+u_I(0,\tau))}{1-\sigma(\varphi_s(\tau)+u_I(0,\tau))}\Big], \quad (21)$$

$$\varphi_s(0) = 0. \quad (22)$$

Since, in this problem, the temperature maximum at the ignition stage is at the point $\xi = 0$, one can conclude on the ignition of the body and obtain the ignition time from the behavior of the heating by chemical reactions $\varphi_s(\tau)$. Problem (21), (22) is a Cauchy problem and is easily solved numerically; there is still one degree of freedom in the choice of the parameter T_*. As was shown in [6], an appropriate choice of T_* results in a weak dependence of the solution on σ. In this problem, as T_*, it is convenient to take the temperature at which the chemical reactions occur near the surface. After $\varphi_s(\tau)$ is found, the burnup is calculated from (20).

We construct the asymptotic solution of problem (21), (22) by the method of matched asymptotic expansions with the use of a large value of the parameter $\Theta_0 \gg 1$, which is typical of the problems of ignition of materials that are able to convert explosively. At the initial stage of the process, $T_s < T_*$, $\varphi_S(\tau)$ is small, and $u_I(0,\tau) \sim o(1)$. Therefore, with accuracy to exponentially small quantities $o(exp(-\Theta_0 u_I(0,\tau)))$, from (21) and (22) we obtain

$$\frac{d\varphi_s(\tau)}{d\tau} = 0, \quad \varphi_s(0) = 0;$$

then we find

$$\varphi_s(\tau) = 0. \quad (23)$$

It follows from (23) that, at the initial stage, the surface temperature varies in the same way as during inert heating, $u(0,\tau) = u_I(0,\tau)$; this corresponds to the solution obtained at the first stage of the adiabatic method [1, 2, 6].

In the process of surface heating, when T_s is close to T_*, we have $u_I(0,\tau) \ll 1$ and $\Theta_0 u_I(0,\tau) \sim o(1)$. At this (second) stage of the process, we use the variables $\tau_1 = \Theta_0(\tau - \tau_0)$ and $\Phi_s(\tau_1) = \Theta_0\varphi_s(\tau)$, where τ_0 is the time when the surface temperature attains T_* and Φ is the heating by chemical reactions in Frank-Kamenetskii's variables. Using the variable τ_1, one can present the solution of the inert problem (6), (7) in the form of the expansion

$$\Theta_0 u_I(0,\tau_1) = A - C_1\tau_1 + o(\Theta_0^{-1}), \quad (24)$$

where A and C_1 are constants of the order of unity. In the new variables, with an accuracy of $o(\Theta_0^{-1})$, Eq. (24) takes the form

$$\frac{d\Phi_s(\tau_1)}{d\tau_1} + \omega\exp[-\Phi_s(\tau_1) - A + C_1\tau_1] = 0. \quad (25)$$

The integration of (25) and its matching with the solution for the initial stage (23) $\Phi_s(\tau_1 \to -\infty) \to 0$ result in

$$\Phi_s(\tau_1) = \ln\Big[1 - \frac{\omega}{C_1}\exp(-A + C_1\tau_1)\Big]. \quad (26)$$

Formula (26) shows the logarithmic variation in the heating at the body surface at the second stage of ignition, which is the same as in the corresponding solution obtained by the adiabatic method [1, 2, 6].

The moment of ignition is defined as the time of unbounded growth of the surface temperature:

$$\Phi_s(\tau_1 \to \tau_{i1}) \to -\infty. \tag{27}$$

This choice of the ignition condition is valid for a reaction of order $m = 0$ and has the asymptotic meaning for $m > 0$. The time for which the surface is heated to T_* is obtained from the condition $T(0, t_0) = T_*$; in dimensionless variables, this condition has the form

$$\Phi_s(0) + \Theta_0 u_I(0, 0) = 0. \tag{28}$$

Since the second stage of the process is considerably shorter than the first stage, similarly to [1, 6], it is convenient to use the extrapolated ignition temperature as the scaling temperature, i.e., the temperature which would be attained by the body surface at the moment of ignition during inert heating:

$$u_I(0, \tau_{i1}) = 0. \tag{29}$$

Substituting (24) and (26) into relations (27)–(29) and solving them, we arrive at the equations

$$A = \ln 2, \quad \omega = C_1, \quad \tau_{i1} = \frac{\ln 2}{C_1}. \tag{30}$$

From (30), using concrete expressions for A and C_1 obtained from the solution of the inert problem (6), (7), we find ω (which determines the scaling temperature T_*), τ_0, and τ_{i1}.

In particular, for a nontransparent body ($B = -\infty$), from (6) and (7) we have $u_I(0, \tau) = 1 - 2\sqrt{\tau/\pi}$; therefore, in the expansion (24), we have

$$A = \Theta_0\Big(1 - 2\sqrt{\frac{\tau_0}{\pi}}\Big), \quad C_1 = \frac{1}{\sqrt{\pi\tau_0}}.$$

Substituting these values of A and C_1 into (30) and solving the resulting system with an accuracy of $o(\Theta_0^{-1})$, we find

$$\omega = \frac{2}{\pi}, \quad \tau_0 = \frac{\pi}{4}, \quad \tau_{i1} = \frac{\pi \ln 2}{2}.$$

In the initial variables of the first heating stage, we obtain the following expression for the ignition time:

$$\tau_i = \frac{\pi}{4} + \frac{\pi \ln 2}{2\Theta_0}. \tag{31}$$

A comparison (in percent) between the ignition time and the result of the numerical calculation of the initial problem (1)–(5) τ_{num} is shown in Table 1 (the first row), where

$$\Delta\tau_i\ [\%] = \frac{\tau_i - \tau_{num}}{\tau_{num}} \cdot 100\%.$$

The minus indicates that the ignition time is approached from below. It is easy to see the asymptotic character of solution (31). The ignition time (31) is in good agreement with the ignition time obtained by the adiabatic method [1]: $\tau_{i,ad} = \pi/4 + \pi/2\Theta_0$,

TABLE 1

B	$\Delta\tau_i$ [%] for Θ_0					
	5	10	20	30	50	100
∞	−23.4	−14.3	−9.2	−7.0	−5.0	−3.1
1.0	−3.8	0.6	0.8	0.6	0.4	0.1
0.1	2.2	3.4	2.3	1.6	1.0	0.5
10.0	−15.2	−5.9	−2.2	−1.1	−0.2	0.5

which also agrees with the result of the numerical calculation.

For a semitransparent body, $B = -\infty$; from (6) and (7), we find

$$u_I(0, \tau) = 1 - 2\sqrt{\frac{\tau}{\pi}} + \frac{1}{B}[1 - \exp(B^2\tau_0)\,\mathrm{erfc}(B\sqrt{\tau_0})];$$

it follows from the expansion (24) that

$$A = \Theta_0\Big\{1 - 2\sqrt{\frac{\tau_0}{\pi}} + \frac{1}{B}[1 - \exp(B^2\tau_0)\,\mathrm{erfc}(B\sqrt{\tau_0})]\Big\},$$

$$C_1 = B\exp(B^2\tau_0)\,\mathrm{erfc}(B\sqrt{\tau_0}).$$

For these constants, system (30) gives

$$1 + B\Big(1 - 2\sqrt{\frac{\tau_0}{\pi}}\Big) = \exp(B^2\tau_0)\,\mathrm{erfc}(B\sqrt{\tau_0}), \tag{32}$$

$$\omega = B\Big[1 + B\Big(1 - 2\sqrt{\frac{\tau_0}{\pi}}\Big)\Big], \tag{33}$$

$$\tau_i = \tau_0 + \frac{\ln 2}{\Theta_0\omega}. \tag{34}$$

For any value of B, Eq. (32) has the only root obtained iteratively:

$$\tau_0^{(i+1)} = \frac{\pi}{4}\Big\{1 + \frac{1}{B}\Big[1 - \exp(B^2\tau_0^{(i)}) \times \mathrm{erfc}\Big(B\sqrt{\tau_0^{(i)}}\Big)\Big]\Big\}^2.$$

For example, for $B = 1$, we obtain $\tau_0 = 2.204$ and, from (33) and (34), we obtain $\omega = 0.325$ and $\tau_i = 2.204 + 2.135/\Theta_0$. For $B = 0.1$, we obtain $\tau_0 = 12.759$ and, from (33) and (34), we obtain $\omega = 0.0697$ and $\tau_i = 12.759 + 9.945/\Theta_0$. A comparison between the ignition time for these values of B and the numerical result of the initial problem (1)–(5) is shown in Table 1 (the second and third rows, respectively). One can see that the asymptotic formulas give the ignition time at the level of accuracy of the numerical calculations. This probably explains the nonmonotonic behavior of the error on the intervals from $\Theta_0 = 10$ to $\Theta_0 = 20$ for $B = 1$ and from

$\Theta_0 = 5$ to $\Theta_0 = 10$ for $B = 0.1$. As can be seen in Table 1, the parameter B affects the way the asymptotic formula approaches the ignition time. For moderate values of B, the asymptotic formula approaches the ignition time from above.

When the parameter B increases, the right side of Eq. (32) decreases rapidly to zero, and, from (32) and (33), we obtain

$$\tau_0 = \frac{\pi}{4}\Big(1 + \frac{1}{B}\Big)^2 + o(B^{-2}),$$

$$\omega = \frac{2}{\pi(1 + 1/B)} + o(B^{-2}), \qquad (35)$$

$$\tau_i = \frac{\pi}{4}\Big(1 + \frac{1}{B}\Big)\Big[1 + \frac{1}{B} + \frac{2\ln 2}{\Theta_0}\Big] + o(B^{-2}).$$

A comparison of the ignition time given by (35) for $B = 10$ with the result of the numerical calculation is shown in the fourth row of Table 1. Quite a good agreement of the results is observed for $\Theta_0 \geqslant 10$.

Conceptually, an asymptotic analysis of the behavior of the temperature of the body surface in the process of ignition by a heat flux is similar to Vilyunov's adiabatic method of obtaining the ignition time. The formulas obtained for the surface temperature and the ignition time are similar to the results of the adiabatic method; they are highly accurate already for real values of Θ_0 and almost coincide with the results of the numerical calculation with increase in Θ_0. Thus, an analysis shows the asymptotic character of the adiabatic method and can be considered as its justification.

As an example, we calculate the dimensional ignition times for a nontransparent and semitransparent nitroglycerin c-substance N: $E = 1.4654 \cdot 10^5$ J/mole, $Q = 1.13 \cdot 10^6$ J/kg, $z = 9.08 \cdot 10^{13}$ sec^{-1}, $\rho = 1.6 \cdot 10^3$ kg/m^3, $c = 1.465 \cdot 10^3$ J/(kg·K), $\lambda = 0.2345$ J/(m·sec·K), $a_0 = 1$, $m = 1$, and $n = 4 \cdot 10^3$ m^{-1}. In this case, $T_0 = 293$ K and $q = 4.1868 \cdot 10^4$ J/(m^2·sec). The addition of 1% of soot makes this c-substance N nontransparent ($n = \infty$). Then, the scaling temperature T_* is obtained from the condition $\omega = 2/\pi$, which yields

$$T_* = \frac{E}{R\ln[\pi Q z \rho^m a_0^m \lambda (T_* - T_0)/(2q^2)]}.$$

This equation has the only root, which can be found, for example, by iterations, and is $T_* = 483.85$ for the specified values of the parameters. Using this value of the scaling temperature, we obtain $\Theta_0 = 14.37$ and $t_h = 11.42$ sec. From (31), we find $t_i = 9.84$ sec.

For a semitransparent c-substance N, Eqs. (32) and (33) and the expressions for ω and B written in terms of dimensional parameters are used to determine T_*. As a result, we arrive at the system solvable by iterations:

$$T_*^{(i)} = \frac{E}{R\{\ln[Qz\rho^m a_0^m/(nq)] - \ln[(\omega/B)^{(i)}]\}},$$

$$B^{(i)} = \frac{n\lambda}{q}(T_*^{(i)} - T_0),$$

$$\tau_0^{(i)} = \frac{\pi}{4}\Big\{1 + \frac{1}{B^{(i)}}\Big[1 - \Big(\frac{\omega}{B}\Big)^{(i)}\Big]\Big\}^2,$$

$$\Big(\frac{\omega}{B}\Big)^{(i+1)} = \exp\Big((B^{(i)})^2\tau_0^{(i)}\Big)\operatorname{erfc}\Big(B^{(i)}\sqrt{\tau_0^{(i)}}\Big).$$

The iterations converge fast and yield $T_* = 481.24$ K, $\tau_0 = 1.146$, $B = 4.217$, and $\omega = 0.515$ for this case. Using the resulting value of T_*, we find $\Theta_0 = 14.32$ and $t_h = 11.083$ sec. Using the calculated quantities, from (34) we find that $t_i = 13.74$ sec. The growth of the ignition time with increase in the transparency of the body is related to the partial penetration of the incoming external heat deep into the body.

For weakly transparent bodies ($B \gg 1$), the scaling temperature and the ignition time are obtained from formulas (35) similarly to the case of a nontransparent body, and, for the c-substance N, we obtain the following values of the parameters: $T_* = 481.23$ K, $\Theta_0 = 14.32$, $B = 4.212$, $t_h = 11.083$ sec, and $t_i = 14.37$ sec. Apparently, the use of formulas (35) is quite acceptable in this case, although the value of B is not very large. The difference in the ignition time is only 4.5%.

The second problem considered here is ignition of a hot spot in a reactive medium. Many researchers studied this problem theoretically; the papers [7–18] are far from a complete list. Using the results of a detailed numerical analysis of the problem [9], Merzhanov [10] showed that the previous approximate theories [11–14] of the critical conditions of thermal explosion of a hot spot are not satisfactory and do not give a correct critical relation between the basic parameters even qualitatively. Basically, the main defect of these theories is connected with an inadequate qualitative treatment of the nonlinear heat production by chemical reactions. This conclusion indicates the need for a more rigorous approach in constructing approximate theories.

In dimensionless variables appropriate inside a heated spot [7, 8], the mathematical formulation of the problem for a plane-parallel initial temperature distribution has the form [9, 16, 18]:

$$\frac{\partial v}{\partial \tau} = \frac{1}{\delta}\frac{\partial^2 v}{\partial \xi^2} - \psi(\eta)\exp\Big(-\frac{v}{1 - \sigma v/\Theta_0}\Big); \qquad (36)$$

$$\frac{\partial \eta}{\partial \tau} = \frac{\mathrm{Le}}{\delta}\frac{\partial^2 \eta}{\partial \xi^2} + \gamma_1\psi(\eta)\exp\Big(-\frac{v}{1 - \sigma v/\Theta_0}\Big), \qquad (37)$$

$$\tau > 0, \quad 0 < \xi < \infty;$$

$$v(\xi,0) = \Theta_0[1 - f(\xi)], \quad \eta(\xi,0) = 0; \tag{38}$$

$$\frac{\partial v(0,\tau)}{\partial \xi} = \frac{\partial \eta(0,\tau)}{\partial \xi} = 0,$$
$$\frac{\partial v(\infty,\tau)}{\partial \xi} = \frac{\partial \eta(\infty,\tau)}{\partial \xi} = 0, \tag{39}$$

where

$$v = \frac{E(T_0 - T)}{RT_0^2}, \quad \eta = \frac{a_0 - a}{a_0}, \quad \xi = \frac{x}{L},$$

$$\tau = \frac{t}{t_{ad}}, \quad \sigma = \frac{T_0 - T_i}{T_0}, \quad \Theta_0 = \frac{E(T_0 - T_i)}{RT_0^2},$$

$$\delta = \frac{\rho^m a_0^m EQzL^2}{\lambda RT_0^2} \exp\Big(-\frac{E}{RT_0}\Big), \quad \mathrm{Le} = \frac{c\rho D}{\lambda},$$

$$\gamma_1 = \frac{cRT_0^2}{a_0 QE}, \quad t_{ad} = \frac{RT_0^2 c}{EQz\rho^{m-1}a_0^m} \exp\frac{E}{RT_0},$$

v is the temperature in Frank-Kamenetskii's variables, $\psi(\eta)$ is the kinetic function of chemical reactions, $f(\xi)$ is a function that defines the initial temperature distribution in the medium with a maximum at the center of the hot spot [$f(0) = 1$ and $f(\infty) = 0$], T_0 and T_i are the initial temperatures at the center of the spot and outside it, and L is the characteristic size (halfwidth) of the hot spot. Then, using, as the dependent variable, the heating by chemical reactions $\Phi = v - v_I$, where v_I is the solution of the problem of inert cooling of a hot spot, we have

$$\frac{\partial v_I}{\partial \tau} = \frac{1}{\delta}\frac{\partial^2 v_I}{\partial \xi^2}, \quad v_I(\xi,0) = \Theta_0[1 - f(\xi)],$$
$$\frac{\partial v_I(0,\tau)}{\partial \xi} = \frac{\partial v_I(\infty,\tau)}{\partial \xi} = 0. \tag{40}$$

From (36)–(39) we obtain

$$\frac{\partial \Phi}{\partial \tau} = \frac{1}{\delta}\frac{\partial^2 \Phi}{\partial \xi^2} - \psi(\eta)\exp\Big[-\frac{\Phi + v_I}{1 - \sigma(\Phi + v_I)/\Theta_0}\Big]; \tag{41}$$

$$\frac{\partial \eta}{\partial \tau} = \frac{\mathrm{Le}}{\delta}\frac{\partial^2 \eta}{\partial \xi^2} + \gamma_1\psi(\eta)\exp\Big[-\frac{\Phi + v_I}{1 - \sigma(\Phi + v_I)/\Theta_0}\Big], \tag{42}$$

$$\tau > 0, \quad 0 < \xi < \infty;$$

$$\Phi(\xi,0) = \eta(\xi,0) = 0; \tag{43}$$

$$\frac{\partial \Phi(0,\tau)}{\partial \xi} = \frac{\partial \eta(0,\tau)}{\partial \xi} = 0,$$
$$\frac{\partial \Phi(\infty,\tau)}{\partial \xi} = \frac{\partial \eta(\infty,\tau)}{\partial \xi} = 0. \tag{44}$$

From problem (41)–(44), which is similar to problem (8)–(11), using Laplace transform with respect to the variable $\xi \to S$ and passing to the limit $S \to \infty$, we obtain the following equations for the heating by chemical reactions and for the burnup at the center of the spot for $\xi = 0$ [$\Phi(0,\tau) = \Phi_s(\tau)$ and $\eta(0,\tau) = \eta_s(\tau)$]:

$$\frac{d\Phi_s}{d\tau} + \psi(\eta_s) \times \exp\Big\{-\frac{\Phi_s + v_I(0,\tau)}{1 - \sigma[\Phi_s + v_I(0,\tau)]/\Theta_0}\Big\} = 0, \tag{45}$$

$$\frac{d\eta_s}{d\tau} - \gamma_1\psi(\eta_s) \times \exp\Big\{-\frac{\Phi_s + v_I(0,\tau)}{1 - \sigma[\Phi_s + v_I(0,\tau)]/\Theta_0}\Big\} = 0, \tag{46}$$

$$\Phi_s(0) = \eta_s(0) = 0. \tag{47}$$

Similarly to (17)–(19), problem (45)–(47) has the first integral $\eta_s(\tau) = -\gamma_1\Phi_s(\tau)$, substitution of which into (45) leads to the problem of heating at the center of the spot:

$$\frac{d\Phi_s}{d\tau} + \psi(-\gamma_1\Phi_s) \times \exp\Big\{-\frac{\Phi_s + v_I(0,\tau)}{1 - \sigma[\Phi_s + v_I(0,\tau)]/\Theta_0}\Big\} = 0, \tag{48}$$

$$\Phi_s(0) = 0. \tag{49}$$

In nondegenerate regimes, at the stage of spot ignition the temperature maximum is at the point $\xi = 0$; therefore, the criterion of ignition and the ignition time can be obtained from Eq. (48). As in the previous problem, for a simple zeroth-order reaction, the moment of ignition can be defined, similarly to [6–8], as the time when the temperature grows unboundedly: $\Phi_s(\tau \to \tau_i) \to -\infty$. For higher-order reactions, this criterion has the asymptotic meaning for $\Theta_0 \gg 1$ and $\gamma_1 \ll 1$. For autocatalytic reactions, the moment of ignition can be defined, similarly to [18], as the time when the maximum rate of the chemical reaction is attained. It is much easier to obtain the ignition time by solving problem (48), (49) numerically than by solving the initial problem (36)–(39). In particular, the numerical calculation of problem (48), (49) yields various regimes of spot ignition, including the regime with initial temperature drop at the center of the spot, which was described in [17], and the critical parameters which separate them.

For materials that are able to convert explosively, one can construct an asymptotic solution of (48), (49) using $\Theta_0 \gg 1$. If the solution of (48), (49) is sought in the form of an asymptotic expansion in the parameter Θ_0^{-1}, then, in the leading approximation, from (48) and (49) we obtain, with accuracy to $o(\Theta_0^{-1})$, the following problem:

$$\frac{d\Phi_s}{d\tau} + \psi(-\gamma_1\Phi_s)\exp[-\Phi_s - v_I(0,\tau)] = 0; \qquad \Phi_s(0) = 0; \tag{50}$$

its integration yields

$$\int_0^{\Phi_s} \frac{\exp y}{\psi(-\gamma_1 y)}dy = -\int_0^{\tau} \exp[-v_I(0,y)]dy. \tag{51}$$

Problem (50) and its integral (51) coincide with the corresponding expressions for spot heating obtained in [7, 16, 18] from an asymptotic analysis for large values of the temperature drop ($\Theta_0 \gg 1$) and Frank-Kamenetskii's parameter ($\delta \gg 1$). For further analysis of (51), it is necessary to clarify the kinetics of the chemical reaction. For an mth-order reaction, we have $\psi(-\gamma_1\Phi) = (1+\gamma_1\Phi)^m$ and, for $\gamma_1 \ll 1$, the integral on the left side of (51) gives

$$\int_0^{\Phi_s} \frac{\exp y}{(1+\gamma_1 y)^m}dy = \frac{\exp\Phi}{(1+\gamma_1\Phi)^m}\left[1 + \frac{\gamma_1 m}{1+\gamma_1 m}\right] - (1+\gamma_1 m) + o(\gamma_1^2). \tag{52}$$

Substitution of (52) into (51) results in a transcendental equation for Φ_s with the only root $\Phi_s < 0$, which can be found by iteration. At the moment of ignition, we have $\Phi_s(\tau \to \tau_i) \to -\infty$, and, from (51) and (52), we obtain the equation for the ignition time:

$$1 + \gamma_1 m = \int_0^{\tau_i} \exp[-v_I(0,y)]dy. \tag{53}$$

The inert cooling of the spot center is determined from (40):

$$v_I(0,\tau) = \Theta_0\sqrt{\frac{\delta}{\pi\tau}} \times \int_0^{\infty}[1 - f(y)]\exp\left(-\frac{\delta y^2}{4\tau}\right)dy. \tag{54}$$

For $\Theta_0 \gg 1$ and bounded values of $\delta \sim o(1)$, the integral in (53) remains less than unity even as $\tau_i \to \infty$, Eq. (53) has no solution, and ignition does not occur. Ignition occurs only for $\delta \gg 1$, when Eq. (53) has a solution. The limiting value δ_*, which separates the stationary and explosive regimes of the process, can be found as is done in [7, 16]. For an U-shaped hot spot, we have $f(\xi) = 1 - \eta(\xi - 1)$; from (54), we find

$$v_I(0,\tau) = \Theta_0 \operatorname{erfc}\left(\frac{1}{2}\sqrt{\frac{\delta}{\tau}}\right) = 2\Theta_0\sqrt{\frac{\tau}{\pi\delta}}\exp\left(-\frac{\delta}{4\tau}\right)\left[1 + o\left(\frac{1}{\delta}\right)\right].$$

Substituting this expression into (53) and expanding the exponential function into a series, we compute the integral with an accuracy to the leading terms and obtain the following equation for the ignition time:

$$\tau_i - (1 + m\gamma_1) = \frac{8\Theta_0\tau_i^{5/2}}{\sqrt{\pi}\delta^{3/2}}\exp\left(-\frac{\delta}{4\tau_i}\right). \tag{55}$$

For $\delta > \delta_*$, this equation has two positive roots, and the smaller one gives the ignition time. The limiting value δ_*, for which the solution still exists, is determined from the tangency condition for the left and right parts of equality (55):

$$\delta_* = 4(1+\gamma_1 m)\left(1 + \frac{4}{\delta_*}\right) \times \ln\left[\frac{2\Theta_0(1+\gamma_1 m)^{5/2}}{\sqrt{\pi\delta_*}}\left(1 + \frac{4}{\delta_*}\right)^{5/2}\right] \tag{56}$$

which is easily solved by iterations. A comparison between the critical value $\delta_*(\Theta_0)$ obtained from (56) for a reaction of order $m = 0$ and the result of the numerical calculation [10] is shown in Table 2, where $\Delta\delta_*$ [%] $= 9(\delta_{*(56)} - \delta_{*[10]})/\delta_{*[10]}) \cdot 100\%$. One can see the asymptotic (for $\Theta_0 \gg 1$) character of the solution. For $\Theta_0 > 40$, the results agree at the level of accuracy of a numerical calculation.

TABLE 2

Θ_0	$\delta_{*[10]}$	$\delta_{*(56)}$	$\Delta\delta_*$, %
10	7.87	10.95	39.1
20	11.07	13.06	18.0
30	13.06	14.35	9.9
40	14.52	15.28	5.2

For the nitroglycerin c-substance N considered in the first problem, the basic parameters entering (56) and (55) are $\Theta_0 = 14.6$ and $\gamma_1 = 1.84 \cdot 10^{-2}$ for $T_0 = 500$ K and $T_i = 293$ K. We obtain the critical value of Frank-Kamenetskii's parameter $\delta_* = 12.35$ from (56), and the ignition time at the boundary of the hot-spot ignition regime $\tau_i = 1.2$ from (55). In dimensional variables, the critical value of the halfwidth of the hot spot and its ignition time are $L = 0.71 \cdot 10^{-4}$ m and $t_i = 0.49$ sec.

CONCLUSIONS

1. Ordinary differential equations for the temperature of the body at the point $x = 0$ for the ignition initiated by a radiation flux and the ignition of a hot spot have been derived. The similarity between heating by means of chemical reactions and burnup at the point $x = 0$ has been demonstrated.

2. An asymptotic analysis of the resulting solutions for large values of the temperature drop ($\Theta_0 \gg 1$) has been carried out, and the results have been compared with the numerical results.

3. An asymptotic analysis of the surface-heating problem (21), (22) upon ignition by a radiation flux has validated Vilyunov's "adiabatic method" of obtaining the temporal ignition characteristics [1, 2, 6].

4. The results of an asymptotical analysis of the ignition of a hot spot [7, 16, 18] have been supported.

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REFERENCES

1. V. N. Vilyunov, "Thermal theory of ignition," *Fiz. Goreniya Vzryva*, **2**, No. 2, 77–82 (1966).
2. V. N. Vilyunov, "Approximate methods for problems of the thermal theory of ignition," in: *Abstracts of the 1st All-Union Symposium on Combustion and Explosion* [in Russian], Nauka, Moscow (1968), pp. 9–11.
3. C. S. Kim and P. M. Chung, "An asymptotic, thermodiffusive ignition theory of porous solid fuels," *J. Heat Transfer*, **98**, 269–276 (1976).
4. C. S. Kim and P. M. Chung, "Ignition of a porous solid fuel by convective heat and mass transfer at the fuel surface," *Combust. Sci. Technol.*, **15**, 75–82 (1977).
5. L. K. Gusachenko, "Heating of the half-space by a penetrating narrow beam," in: *Methods and Algorithms of Parametric Analysis of Nonlinear Transfer Models* [in Russian], No. 6, MGOPI, Moscow, (1988), pp. 22–27.
6. V. N. Vilyunov, *Theory of Ignition of Condensed Materials* [in Russian], Nauka, Novosibirsk (1987).
7. R. S. Burkina and V. N. Vilyunov, "Initiation of a chemical reaction at a hot spot," *Fiz. Goreniya Vzryva*, **16**, No. 4, 75–79 (1980).
8. R. S. Burkina and V. N. Vilyunov, *Asymptotic Behavior of the Problems of Ignition Theory* [in Russian], Izd. Tomsk Univ., Tomsk (1982).
9. A. G. Merzhanov, V. V. Barzykin, and V. T. Gontkovskaya, "The problem of thermal explosion of a hot spot," *Dokl. Akad. Nauk SSSR*, **148**, No. 2, 380–383 (1963).
10. A. G. Merzhanov, "Critical conditions for thermal explosion of a hot spot," *Combust. Flame*, **10**, No. 4, 341–348 (1966).
11. J. Zinn, "Initiation of explosions of hot spots," *J. Chem. Phys.*, **36**, No. 7, 1949 (1962).
12. T. Boddington, "The growth and decay of hot spots and the relation between structure and stability," in: *9th Symp. on Combustion*, Academic Press, New York (1963), p. 287.
13. M. H. Friedman, "Size of hot spots in the impact explosion of exothermic materials," *Trans. Faraday Soc.*, **59**, No. 8, 1865 (1963).
14. P. H. Thomas, "A comparison of some hot spot theories," *Combust. Flame*, **9**, No. 4, 369–372 (1965).
15. P. H. Thomas, "An approximate theory of 'hot spot' critically," *Combust. Flame*, **21**, No. 1, 99–109 (1973).
16. R. S. Burkina and V. N. Vilyunov, "Thermal ignition of a hot spot for an arbitrary initial temperature distribution," *Khim. Fiz.*, No. 3, 419–422 (1982).
17. A. G. Knyazeva, R. S. Burkina, and V. N. Vilyunov, "Specifics of thermal ignition of a hot spot for various initial temperature distributions," *Fiz. Goreniya Vzryva*, **24**, No. 3, 45–47 (1988).
18. R. S. Burkina and A. G. Knyazeva, "The effect of autocatalysis on thermal ignition of a hot spot," *Fiz. Goreniya Vzryva*, **27**, No. 2, 15–21 (1991).