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Theoretical studies [1-3], concerning the ignition of reacting substances, deal with ignition by a heated infinite plate. However, actual igniters have finite dimensions and a nonzero mean surface curvature. Moreover, under actual conditions, in addition to unilateral heating of the reacting substance, there is heat transfer to the ambient medium.

This study, following [4], employs the methods of Shvets [5] and integral relations [6] to evaluate the effect of these factors on the process of ignition of a reacting substance.

§1. We will consider the ignition of a reacting substance by a heated cylinder. We neglect burnup and assume that the thermophysical coefficients are constants, which makes the heat capacity of the cylinder infinitely large. Then, mathematically, the problem reduces to solving

$$\frac{\partial^2\theta}{\partial x^2} = \delta\frac{\partial\theta}{\partial\tau} - \frac{1}{x}\frac{\partial\theta}{\partial x} - \delta e^\theta \quad \left(\delta = \frac{qk_0 r_0^2 E}{\lambda R T_*^2}\exp - \frac{E}{RT_*}\right), \tag{1.1}$$

with boundary and initial conditions

$$\theta(1,\tau) = 0, \quad \theta(\infty,\tau) = -\theta_0, \quad \theta(x,0) = -\theta_0 \tag{1.2}$$

$$\left(x = \frac{r}{r_0},\ \theta = \frac{(T - T_*)E}{RT_*^2},\ \theta_0 = \frac{(T_* - T_0)E}{RT_*^2},\right.$$

$$\left.\tau = \frac{qk_0 Et}{c\rho RT_*^2}\exp - \frac{E}{RT_*}\right).$$

Here, x is the dimensionless variable radius; r_0 is the cylinder radius; δ is a dimensionless parameter, τ is a dimensionless time, q is the reaction energy; λ is the thermal conductivity; E is the activation energy; R is the universal gas constant; t is time; T_* is the temperature of the heated cylinder; T_0 is the initial temperature of the reactant. θ is a dimensionless temperature; ρ is density; c is specific heat; k_0 is the preexponential factor.

In deriving Eq. (1.1) the Frank-Kamenetskii transformation [7] for exp − E/RT was employed.

Boundary-value problem (1.1) and (1.2) describes the ignition of a reactant by a heated wire which is instantaneously heated to a temperature T_* which remains unchanged up to the moment of ignition. With a certain condition [3] this problem also describes the ignition of reacting substances for first-order reactions.

Since, under actual conditions, the wire is heated gradually and has a finite heat capacity and the reactant is consumed, the heating time found from (1.1) and (1.2) will be less than the true value.

By virtue of the exponential temperature dependence of the chemical reaction rate, an intense temperature change occurs in a narrow boundary layer at the heated surface. Accordingly, it is desirable to introduce the thickness of the boundary layer $\Delta = \Delta(\tau)$. Then boundary and initial conditions (1.2) take the form:

$$\theta(1,\tau) = 0, \quad \theta(1+\Delta,\tau) = -\theta_0, \quad \Delta(0) = 0. \tag{1.3}$$

To solve (1.1) and (1.3) we use the method of Shvets [5], which, apart from its simplicity, has good convergence [8]. As the first approximation for the temperature we obtain

$$\theta_1 = -\frac{\theta_0(x-1)}{\Delta}. \tag{1.4}$$

Substituting (1.4) into the right side of (1.1), integrating the result twice with respect to x, and using (1.3), we have

$$\theta_2 = \frac{\theta_0 x}{\Delta}(\ln x - 1) + \frac{\delta\theta_0\Delta^{\cdot}}{6\Delta^2}[2 - 3x^2 + x^3 + (1-x)(\Delta^2 - 3)] +$$
$$+ \frac{\delta\Delta^2}{\theta_0^2}\left[1 - \exp\frac{\theta_0(1-x)}{\Delta}\right] + \frac{\delta\Delta}{\theta_0^2}(1-x) + \frac{\theta_0(2-x)}{\Delta} + \tag{1.5}$$
$$+ \frac{\theta_0}{\Delta^2}\{1 + (1+\Delta)[\ln(1+\Delta) - 1]\}(1-x).$$

Satisfying Shvets's condition $\partial\theta/\partial x = 0$ at $x = \Delta$ [5], we obtain a first-order differential equation for $\Delta(\tau)$:

$$\delta\Delta\Delta^{\cdot} = \frac{3\ln(1+\Delta)}{\Delta} + \frac{3\delta\Delta^2}{\theta_0^3}. \tag{1.6}$$

Satisfying the Zel'dovich condition $\partial\theta/\partial x = 0$ at $x = 0$ [9], we find

$$\delta\Delta\Delta^{\cdot} = \frac{6\delta(\theta_0 - 1)\Delta^2}{\theta_0^3} - \frac{6(1+\Delta)\ln(1+\Delta)}{\Delta}. \tag{1.7}$$

Eliminating the quantity $\delta\Delta\Delta^{\cdot}$, from Eq. (1.6) and (1.7), we obtain

$$\delta = \frac{\theta_0^3(3 + 2\Delta_*)\ln(1+\Delta_*)}{(2\theta_0 - 3)\Delta_*^3}. \tag{1.8}$$

Solving Eq. (1.8), we find the thickness of the heated layer Δ_*. Knowing Δ_*, we easily obtain the heating time

$$\tau_* = \frac{\delta}{3}\int_0^{\Delta_*}\frac{\Delta^2 d\Delta}{\ln(1+\Delta) + \delta\theta_0^{-3}\Delta^3}. \tag{1.9}$$

In the limit as $\delta \to \infty$, from (1.5) and (1.9), we obtain the temperature profile and the heating time for ignition by a heated plate.

From (1.5) and (1.6) it is easy to see that at moderate values the perturbation of temperature profile and boundary-layer thickness due to the heat of the chemical reaction is small. In particular, as $\delta \to \infty$ the perturbation is small at $0 < \tau \le \tau_*$. Since convergence of Shvets's method [5] in the solution of linear boundary-value problems has been proved by Gandin [8], while the perturbation due to the heat of reaction is small, it may be assumed that the successive approximations converge in our case too, at least for $\delta \gg 1$, $\theta_0 \gg$ and $0 < \tau \le \tau_*$. In particular, for small values of τ the error of approximate solution (1.5) does not exceed 8%.

From (1.9) it is clear that τ_* depends significantly on δ; δ is the square of the reduced characteristic dimension. It is clear from (1.6) that for any $\Delta > 0$ the quantity $\Delta > 0$ and, consequently, the greater τ, the greater the thickness of the boundary layer. As follows from (1.8), at small Δ_* the quantity δ tends to infinity, and falls as Δ_* increases, approaching 0 as $\Delta_* \to \infty$. Conversely, large values of δ correspond to smaller values of Δ_*. Consequently, from this analysis it follows that as δ decreases the heating time increases, and conversely.

Thus, the greater the reduced characteristic dimension of the body, the shorter is the heating time and, consequently, the more easily the reacting substance is ignited.

At very large values of δ it is possible, using the method of a small parameter [10], to find an approximate solution of Eq. (1.6) with initial condition (1.3).

By setting

$$u = u_0 + \frac{u_1}{\sqrt{\delta}} + \frac{u_2}{\sqrt{\delta}} + \cdots \quad (u = \delta\Delta^2) \tag{1.10}$$

and substituting (1.10) in (1.6), we obtain

$$u_0^{\cdot} - \frac{6u_0}{\theta_0^3} = 6,\ u_0(0) = 0;$$
$$u_1^{\cdot} - \frac{6u_1}{\theta_0^3} = -3\sqrt{u_0},\ u_1(0) = 0. \tag{1.11}$$

Solving the Cauchy problems (1.11), we find

$$u_0 = \theta_0^3(p - 1),$$

$$u_1 = \tfrac{1}{2}\theta_0^{3/2}[\sqrt{p-1} - p\,\mathrm{arc\,tg}\sqrt{p-1}]\ \left(p = \exp\frac{6\tau}{\theta_0^3}\right). \tag{1.12}$$

Thus, using (1.10) and (1.12) we can determine the value of u correct to terms containing the quantity δ^{-1} as a factor.

Substituting the value of u obtained in (1.8) and solving the resulting equation by the method of a small parameter [11] for τ, we find

$$\tau_* = \frac{\theta_0^3}{6}\ln\frac{2\theta_0}{2\theta_0 - 3}\left\{1 + \frac{1}{2}\left(\frac{\theta_0^3}{\delta}\right)^{1/2}\left[\mathrm{arc\,tg}\left(\frac{3}{2\theta_0 - 3}\right)^{1/2} - \right.\right.$$

$$- (1 - 2\theta_0^{-1}) \left(\frac{3}{2\theta_0 - 3}\right)^{1/2} \Big]\Big\}. \tag{1.13}$$

It is clear from (1.13) that as $\delta \to \infty$ heating time decreases asymptotically, tending to the value obtained for ignition by a plate [12]

$$\tau_* = \frac{\theta_0^3}{6} \ln \frac{2\theta_0}{2\theta_0 - 3} \approx \frac{\theta_0^2}{4} + \frac{3\theta_0}{16} \qquad (\theta_0 \gg 1). \tag{1.14}$$

Comparing (1.14) with the formula for τ_* obtained in [3] on a computer, we see that the heating time determined from (1.14) almost coincides with the results of the numerical calculation [3].

Equation (1.13) is the more accurate, the larger δ. In particular, when $\theta_0 = 10$, $\delta = 3.244$ and $\delta = 4335.6$ we have $\Delta_* = 0.204$; integrating (1.9) by Simpson's rule for ten ordinates [11], we find $\tau_* = 111.5$ and $\tau_* = 29.5$, and from (1.13) we obtain $\tau_* = 108.7$ and $\tau_* = 29.6$, respectively.

Thus, the effect of the surface curvature and finite dimensions of the heated body are the more important, the smaller δ.

§2. We consider the ignition of a reacting substance by a heated sphere on the assumption that the thermophysical coefficients are constant and the reaction is zero-order. The problem reduces to the solution of the equation

$$\frac{\partial^2\theta}{\partial x^2} = \delta \frac{\partial\theta}{\partial\tau} - \frac{2}{x}\frac{\partial\theta}{\partial x} - \delta e^\theta \tag{2.1}$$

with boundary and initial conditions (1.3).

As before, as the first approximation for $\theta(x, \tau)$ we obtain (1.4). Omitting the intermediate calculations, which are similar to those already presented, we write the final results:

$$\theta_2 = \frac{2\theta_0 x}{\Delta}(\ln x - 1) + \frac{\delta\theta_0\Delta^\cdot}{6\Delta^2} \times$$
$$\times [2 - 3x^2 + x^3 + (1 - x)(\Delta^2 - 3)] + \frac{\delta\Delta(1 - x)}{\theta_0^2} + \tag{2.2}$$
$$+ \frac{\delta\Delta^2}{\theta_0^2}\left[1 - \exp\frac{\theta_0(1 - x)}{\Delta}\right] + \frac{\theta_0(3 - x)}{\Delta} +$$
$$+ \frac{2\theta_0}{\Delta^2}\{1 + (1 + \Delta)[\ln(1 + \Delta) - 1]\}(1 - x); \tag{2.3}$$

$$\delta\Delta\Delta^\cdot = \frac{3\delta\Delta^2}{\theta_0^3} + 3\left[\frac{2\ln(1 + \Delta)}{\Delta} - 1\right], \qquad \Delta(0) = 0;$$
$$\delta = \frac{\theta_0^3[2(3 + 2\Delta_*)\ln(1 + \Delta_*) - 3\Delta_*]}{(2\theta_0 - 3)\Delta_*^3}; \tag{2.4}$$

$$\tau_* = \frac{\delta}{3}\int_0^{\tau_*} \frac{\Delta^3 d\Delta}{3\ln(1 + \Delta) - \Delta + \delta\theta_0^{-3}\Delta^3}. \tag{2.5}$$

Here and above, we have omitted terms containing the quantity $\varepsilon = e^{-\theta_0}$ as factor.

From (2.3) it is easy to establish that at $\Delta < 1$ the quantity increases with increase in τ, while from Eq. (2.4) we find that as δ increases the quantity Δ_* decreases; consequently, the smaller δ, the greater is the heating time, and conversely. For large values of δ we can use the small parameter method to find an approximate solution of Cauchy problem (2.3):

$$u = \theta_0^3\left\{p - 1 + \left(\frac{\theta_0^3}{\delta}\right)^{1/2}[\sqrt{p-1} - p \operatorname{arc\,tg}\sqrt{p-1}]\right\}. \tag{2.6}$$

Substituting (2.6) into (2.4) and solving the equation obtained by the small parameter method for τ, we find an approximate analytic expression for the heating time:

$$\tau_* = \frac{\theta_0^3}{6}\ln\frac{2\theta_0}{2\theta_0 - 3}\left\{1 + \left(\frac{\theta_0^3}{\delta}\right)^{1/2} \times\right.$$
$$\left.\times\left[\operatorname{arc\,tg}\left(\frac{3}{2\theta_0 - 3}\right)^{1/2} - (1 - 2\theta_0^{-1})\left(\frac{3}{2\theta_0 - 3}\right)^{1/2}\right]\right\}. \tag{2.7}$$

This equation is the more accurate, the larger δ.

Comparing (1.13) and (2.7), we see that at the same values of δ and θ_0 the value of (2.7) is greater than that of (1.13).

Thus, if a cylinder of a certain radius is heated to a certain temperature and ignites a reacting gas, the gas will not be ignited by a sphere of the same radius heated to the same temperature. This is because at the same radii themean curvature of the sphere is greater than thatof a cylindrical surface. Calculation of τ_* by numerical integration of (2.5) confirms this conclusion. Thus, for $\theta_0 = 10$, $\delta = 4335.6$ and $\Delta_* = 1/4$, from (2.5) we find $\tau_* = 31.4$, which exceeds the time for ignition by a cylinder by a factor of 1.06.

The heating time is uniquely related to the temperature of the heated body. Since the heating time decreases as the characteristic dimension increases, the temperature of the heated surface at which ignition takes place (ignition temperature) also decreases with increase in the characteristic dimension, tending asymptotically to the ignition temperature of a heated plate. This conclusion is consistent with the experimental data of [13].

In conclusion we note that the solution of problems (1.1), (1.3) and (2.1), (1.3) by the Shvets method [5] is the more accurate, the smaller Δ compared with unity.

§3. In order to estimate the effect of heat transfer to the ambient medium, we will consider the case of ignition from the end face of a reacting semi-infinite cylinder. It is assumed that a constant temperature T_0 is maintained at the lateral surface of the cylinder, which will be the case if the reacting substance is enclosed in a vessel whose walls have a large heat capacity or when the reacting substance is subjected to intense cooling by a fluid. Mathematically, the problem reduces to the solution of

$$\delta x\frac{\partial\theta}{\partial\tau} = x\frac{\partial^2\theta}{\partial z^2} + \frac{\partial}{\partial x}\left(x\frac{\partial\theta}{\partial x}\right) + \delta x e^\theta \tag{3.1}$$

with boundary and initial conditions:

$$\theta(\tau, x, 0) = -\theta_0 x^2, \ \theta(\tau, x, \Delta) = -\theta_0,$$
$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0} = 0, \ \theta(\tau, 1, z) = -\theta_0, \ \Delta(0) = 0. \tag{3.2}$$

Here, $z = z_1/r_0$ is the dimensionless axial coordinate.

In deriving (3.1) we employed the Frank-Kamenetskii transformation [7] for exp – E/RT and in deriving (3.2) we introduced the thicknessof the temperature boundary layer.

We will solve boundary-value problem (3.1) and (3.2) by means of a combination of Shvets's method [5] and the method of integral relations [6]. We integrate (3.1) with respect to x from 0 to 1, substituting

$$\theta \approx w(\tau, z)(1 - x^2) - \theta_0 x^2,$$
$$e^\theta \approx (1 - x^2)e^w + \varepsilon x^2, \ (w = \theta(\tau, 0, z)). \tag{3.3}$$

As a result we obtain the equation

$$\partial^2 w / \partial z^2 = \delta\partial w / \partial\tau + 8(w + \theta_0) - \delta(e^w + \varepsilon) \tag{3.4}$$

with boundary and initial conditions:

$$w(\tau, z) = 0, \quad w(\Delta, \tau) = -\theta_0, \quad \Delta(0) = 0. \tag{3.5}$$

We solve (3.4) and (3.5) by Shvets's method [5]. As the first approximation we obtain

$$w_1 = -\theta_0 z / \Delta. \tag{3.6}$$

Substituting w_1 in the right side of (3.4) and integrating the result twice with respect to z, using the first and second conditions of (3.5) we find

$$w_2 = \frac{\delta\theta_0\Delta^\cdot z^3}{6\Delta^2} - \frac{4\theta_0 z^3}{3\Delta} + 4\theta_0 z^2 + \frac{\delta\Delta^2}{\theta_0^2}\left[1 - \exp\left(-\frac{\theta_0 z}{\Delta}\right)\right] -$$
$$- \frac{z}{\Delta}\left(\theta_0 + \frac{8\theta_0\Delta^2}{3} + \frac{\delta\Delta^2}{\theta_0^2} + \frac{\delta\theta_0\Delta\Delta^\cdot}{6}\right). \tag{3.7}$$

Satisfying Shvets's condition [5], we obtain an equation for

$$\delta\Delta\Delta^\cdot = \Delta^2(3\delta / \theta_0^3 - 4) + 3. \tag{3.8}$$

Integrating (3.8) with allowance for the last conditions of (3.5), we find

$$\tau = \frac{\delta}{6b}\ln(1 + b\Delta^2),$$
$$\Delta^2 = \frac{1}{b}\left(\exp\frac{6b\tau}{\delta} - 1\right) \quad \left(b = \frac{\delta}{\theta_0^3} - \frac{4}{3}\right). \tag{3.9}$$

It is clear from (3.7) and (3.8) that at moderate values of τ the perturbation of temperature profile and boundary-layer thickness is small. In the absence of reaction heat the temperature gradient at $x = 0$, found by Shvets's method [5], differs from the corresponding exact values [14] by 8% at τ and by 22% at $\tau \gg 1$. By means of the solution for the problem of thermal explosion in an infinite cylinder it hasbeen established that approximation (3.3) and averaging all the quantities with respect to x introduces an error ≈11%.

Thus, it may be provisionally assumed that the greatest error to be expected in solving boundary-value problem (3.1) and (3.2) by a combination of the Shvets method [5] and the method of integral relations [6] does not exceed 22%.

Making (3.7) satisfy the Zel'dovich condition [9] and using the first expression of (3.9) we obtain the heating time

$$\tau_* = \frac{\delta\theta_0^3}{2(4\theta_0^3 - 3\delta)} \ln \frac{\delta(2\theta_0 - 3) - 4\theta_0^3}{2\theta_0(\delta - 4\theta_0^2)} \tag{3.10}$$

and using the second expression of (3.9), the thickness of the boundary layer

$$\Delta_* = \theta_0 \left(\frac{3\theta_0}{\delta(2\theta_0 - 3) - 4\theta_0^3} \right)^{1/2}. \tag{3.11}$$

From (3.10) it is easy to see that as

$$\delta \to \delta_* = 4\theta^2, \tag{3.12}$$

the quantity $\tau_* \to \infty$, i.e., ignition does not take place.

If the heat transfer from the lateral surface of the reacting cylinder is governed by Newton's law, then, similarly, we find

$$\begin{gathered}\tau_* = \frac{8\theta_0^3(4+B)}{6m(4+B)[1+(\gamma-\varepsilon-\varepsilon n\theta_0)n^{-2}] - 4B\theta_0^3} \times \\ \times \ln \frac{2\theta_0\{m(4+B)[1+(\gamma-\varepsilon)n^{-1}] - 4B\theta_0^2\}}{m(4+B)\{2\theta_0 - 3 + [n\theta_0(2\gamma+\varepsilon) + 3(\varepsilon-\gamma)]n^{-2}\} - 4B\theta_0^3}\end{gathered} \tag{3.13}$$

It is easy to see that the heating tends to infinity if

$$\begin{gathered}\delta \to \delta_* = \frac{8B\theta_0^2}{(2+B)[2+(\gamma-\varepsilon)(2+B)]} \times \\ \times \left(m = \frac{\delta(2+B)}{4+B},\ n = \frac{2}{2+B},\ \gamma = \exp - \frac{B\theta_0}{2+B} \right)\end{gathered} \tag{3.14}$$

Here, $B = \alpha r_0/\lambda$ is the Biot number, α the heat transfer coefficient, and r_0 the radius of the cylinder.

As $B \to \infty$ (3.12) follows from (3.14), and as $B \to 0$ or $m \to \infty$ from expression (3.13) we obtain the heating time for ignition by a heated plate (1.14). We obtain the same results from (3.10) as $\delta \to \infty$.

Thus, to obtain ignition of a reacting cylinder from the end face in the presence of Newtonian heat transfer from the lateral surface, it is necessary for δ to be greater than δ_*, where δ_* is given by (3.14).

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