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ON IGNITING A REACTING GAS BY A HEAT SOURCE OF FINITE HEAT CAPACITY

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The problem of igniting gas by a body of finite heat capacity is solved by the method of joining asymptotic expansions and, also, by numerical methods, taking into account the reagent burnout and variation of heater temperature. The space-time pattern of temperature distribution is determined, and the law of the igniter temperature variation established. Dependence of the ignition time on characteristic parameters of the problem, such as the order of reaction, the Lewis and activation numbers, thermophysical parameters of the heater, etc. is established. It is assumed in the analysis that ignition takes place when the heat flux through the igniter surface becomes zero. Results of numerical solution of the input problem are compared with the approximate analytical determination. It is established that for $\beta = E / (RT_0)$ of order 20 they differ by not more than 15 – 20%; with increasing β the difference diminishes.

The problem of igniting a reacting medium by heat was considered in [1 – 8], using various analytical [1, 3 – 8] and numerical [2] methods.

1. Statement of the problem. The one-dimensional problem of igniting gas by means of a heated plate of finite thickness is defined on the usual simplifying assumptions (see, e.g. [9]) by the following system of equations and boundary conditions:

$$\rho_2 c_2 \frac{\partial T_2}{\partial t'} = \frac{\partial}{\partial z}\left(\lambda_2 \frac{\partial T_2}{\partial z}\right) - mc_2 \frac{\partial T_2}{\partial z} + Q\Phi(y, T_2) \qquad (1.1)$$

$$\rho_2 \frac{\partial y}{\partial t'} = \frac{\partial}{\partial z}\left(D\rho_2 \frac{\partial y}{\partial z}\right) - m\frac{\partial y}{\partial z} + \Phi(y, T_2)$$

$$dT_1 / dt' = \lambda_1 (c_1\rho_1 R_0)^{-1} (\partial T_2 / \partial z)_{z=R_0}$$

$$\partial\rho_2 / \partial t' + \partial m / \partial z = 0, \quad T_2\rho_2 = \text{const}$$

$$z = R_0,\ T_2(R_0, t') = T_1(R_0, t'),\ \partial y / \partial z = 0\ (m(z = R_0, t') = 0)$$

$$z = \infty,\ T_2(\infty, t') = T_-,\ y(\infty, t') = 0$$

$$t' = 0,\ T_2(z, 0) = T_-,\ y(z, 0) = 0,\ T_1(0) = T_0$$

where t' is the time, z is the space coordinate, R_0 is a characteristic dimension of the heated body, T_1 is the temperature of the inert body, T_2 is the temperature of gas, y is the mass portion of the reaction product, n is the order of reaction, λ_i, c_i and ρ_i are the thermal conductivity, specific heat, and density of the inert body $(i = 1)$ and of gas $(i = 2)$, Q is the reaction heat effect, k is the preexponential factor, R is the universal gas constant, E is the activation energy, T_- is the initial temperature of gas, and T_0 the initial temperature of the body $((T_0 - T_-) E / (RT_0^2) \gg 1)$.

It is assumed that for the existence of solution the heat emission function is nonzero everywhere, except in the small temperature interval $T_- \leqslant T < T_\varepsilon$, where it is zero [9], and is determined by the formula

$$\Phi = k\rho_2^n (1 - y)^n \exp [- E / (RT_2)]$$

In the heat balance equation of the igniting plate the temperature distribution inside it is assumed uniform, i.e. $T_1 (z, t') = T_1 (t)$, which is fully justified when the thermal diffusivity of the body $\lambda_1 / (\rho_1 c_1)$ is fairly high.

We pass from variables (t', z) to variables (t', ψ) using formulas

$$m = - \partial\psi / \partial t', \quad \rho_2 = \partial\psi / \partial z, \quad \psi (z = R_0, t') = 0 \tag{1.2}$$

In the new variables the equation of continuity is identically satisfied. The remaining relations in (1.1) assume in dimensionless variables the form

$$\frac{\partial\theta}{\partial t} = \frac{\partial^2\theta}{\partial X^2} + \beta (1 - y)^n \Gamma (\theta) \exp [\beta (\theta - 1) / (\theta + \sigma)] \tag{1.3}$$

$$\frac{\partial y}{\partial t} = L^{-1} \frac{\partial^2 y}{\partial X^2} + \beta\gamma (1 - y)^n \Gamma (\theta) \exp [\beta (\theta - 1) / (\theta + \sigma)]$$

$$\partial a / \partial t = \alpha (\partial\theta / \partial X)_{X=0}$$

$$X = 0, \ \theta (0, t) = a (0, t), \quad \partial y / \partial X = 0$$

$$X = \infty, \ \theta (\infty, t) = 0, \ y (\infty, t) = 0$$

$$t = 0, \ \theta (X, 0) = 0, \ a (0) = 1$$

$$\theta = (T_2 - T_-) / (T_0 - T_-), \quad \sigma = T_- / (T_0 - T_-), \quad \beta = (E / RT_0)$$

$$X = \psi / \Delta x, \ t = t' / \Delta t, \ \gamma = c_2 (T_0 - T_-) / Q$$

$$(\Delta x)^2 = \lambda_2 \Delta t \rho_2 / c_2, \ \Delta t = \beta\gamma / [\rho_0^{n-1} k \exp (- \beta)], \ L = \lambda_2 / (D \rho_2 c_2)$$

$$\alpha = \lambda_1 \rho_2 \Delta t / (c_1 \rho_1 R_0 \Delta x), \quad a = (T_1 - T_-) / (T_0 - T_-), \quad \Gamma (\theta) = (\rho / \rho_0)^{n-1}, \ \rho_0 = \rho (T_0)$$

where it is assumed that $D\rho_2^2$ and $\lambda_2\rho_2 = \text{const}$, since usually $D \sim T^2$, $\rho \sim 1 / T$ and $\lambda \sim T$; and $c_2 = \text{const}$. As units of the space coordinate and of time we select the characteristic thickness of the zone of the steady combustion wave warm-up, and the characteristic time of the steady comubustion wave warm-up, respectively,

2. **Solution of the problem.** Problem (1.3) will be solved by numerical and approximate analytical methods. In the analytical investigation the method of joining asymptotic expansions is used on the assumption of considerable activation energies $(\beta \gg 1)$. The instant at which the heat flux from the heater to the gas vanishes is taken as the instant of ignition. The approximate solution of problem (1.3) is sought in the form of sum

$$\theta (X, t) = \Theta_i (X, t) + u (X, t) \tag{2.1}$$

where function Θ_i defines the stage of passive warm-up, i.e.

$$\partial\theta_i \,/\, \partial t = \partial^2\theta_i \,/\, \partial X^2 \tag{2.2}$$

The solution of problem (2.2) is of the form

$$\Theta_i = \frac{X}{2\sqrt{\pi}} \int_0^t \frac{\exp\left[-X^2/(4(t-\tau))\right]}{(t-\tau)^{3/2}}\, a(\tau)\, d\tau \tag{2.3}$$

After substitution of (2.1) into (1.3) we obtain

$$\begin{aligned}
&\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial X^2} + \beta(1-y)^n \Gamma(\theta) \exp\left(\frac{\beta(\theta_i + u - 1)}{\theta_i + u + \sigma}\right) \\
&\frac{\partial y}{\partial t} = L^{-1}\frac{\partial^2 y}{\partial X^2} + \beta\gamma(1-y)^n \Gamma(\theta) \exp\left(\frac{\beta(\theta_i + u - 1)}{\theta_i + u + \sigma}\right) \\
&\frac{da}{dt} = \alpha\left[\left(\frac{\partial\theta_i}{\partial X}\right)_{X=0} + \left(\frac{\partial u}{\partial X}\right)_{X=0}\right] \\
&u(0, t) = u(\infty, t) = u(X, 0) = 0 \\
&y(\infty, t) = 0, \ (\partial y/\partial X)_{X=0} = 0, \ y(X, 0) = 0 \\
&a(0) = 1
\end{aligned} \tag{2.4}$$

In the interval $0 \leqslant X \leqslant \infty$ of variation of the variable we separate the region adjacent to the heated plate surface (the boundary layer) in which we introduce the variable $x = \beta X$. The term which defines the chemical reaction in the outer region is exponentially small.

We seek the solution of problem (2.4) in the inner and outer regions in the form of expansions

$$\begin{aligned}
&u(X, t) = \beta^{-1}u_1(x, t) + \beta^{-2}u_2(x, t) + O(\beta^{-3}) \\
&y(X, t) = y_0(x, t) + \beta^{-1}y_1(x, t) + O(\beta^{-2}) \\
&a(t) = 1 + \beta^{-1}a_1(t) + O(\beta^{-2})
\end{aligned} \tag{2.5}$$

$$\begin{aligned}
&u(X, t) = \beta^{-1}v_1(X, t) + \beta^{-2}v_2(X, t) + O(\beta^{-3}) \\
&y(X, t) = Y_0(X, t) + \beta^{-1}Y_1(X, t) + O(\beta^{-2})
\end{aligned} \tag{2.6}$$

In each of these regions the asymptotic expansions (2.5) and (2.6) must satisfy the initial and boundary conditions. Congruence between the regions is established by the condition of joining [10, 11].

For the principal terms of expansion in the inner region from (2.4) – (2.6) we have

$$\partial^2 u_1/\partial x^2 + (1 - y_0)^n \exp\left(\frac{a_1 + u_1 - x/\sqrt{\pi t}}{1+\sigma}\right) = 0 \tag{2.7}$$

$$\partial^2 y_0/\partial x^2 = 0 \tag{2.8}$$

$$da_1/dt = \alpha_0\left[-(\pi t)^{-1/2} + (\partial u_1/\partial x)_{x=0}\right] \tag{2.9}$$

$$u_1(0, \tau) = u_1(x, 0), \ (\partial y_0/\partial x)_{x=0} = 0, \ a_1(0) = 0$$

It follows from Eq. (2.8) and the boundary condition at $x = 0$ that $y_0 = y_0(t)$. The general solution of Eq. (2.7) is of the form

$$u_1(x, t) = x / \sqrt{\pi t} - a_1(t) + (1 + \sigma)[-n \ln(1 - y_0) + \ln C_2 - 2 \ln \mathrm{ch}(C_1 + x \sqrt{C_2 / (2(1 + \sigma))})] \quad (2.10)$$

and the boundary condition for $u_1(0, t)$ yields

$$u_1(0, t) = -a_1(t) + (1 + \sigma)[-n \ln(1 - y_0) + \ln C_2 - 2 \ln \mathrm{ch}\, C_1] = 0 \quad (2.11)$$

$$\mathrm{ch}^2 C_1 = (1 - y_0(t))^n \exp(-a_1(t)/(1 + \sigma)) C_2(t)$$

For the temperature gradient at the igniter surface from formula (2.10) we obtain

$$(\partial\theta/\partial x)_{x=0} = -(\pi t)^{1/2} F(t) \quad (2.12)$$

$$F(t) = [1 - 2\pi(1 + \sigma) t (1 - y_0)^n \exp(a_1/(1 + \sigma))]^{1/2}$$

which shows that the heat flux vanishes when the radicand of (2.12) becomes zero. At that instant the inert body is transformed from a source to a sink; in accordance with the definition given above, we take this instant as the instant of ignition. The equation for the determination of the instant of ignition is of the form $F(t) = 0$ (in the second of formulas (2.12) $y_0(t)$ and $a_1(t)$ are unknown functions).

Taking into account (2.12) we represent Eq. (2.9) in the form

$$da_1/dt = -\alpha_0 (\pi t)^{-1/2} F(t) \quad (2.13)$$

For joining the principal terms of the inner and outer expansions (2.5) and (2.6), respectively, from (2.10) we have the following asymptotic expression for u_1 with $x \to \infty$:

$$u_1(x \to \infty, t) = x[(\pi t)^{-1/2} - (2(1 + \sigma) C_2)^{1/2}] + f(t) + O(1) \quad (2.14)$$

$$f(t) = (1 + \sigma)[-n \ln(1 - y_0) + \ln C_2 - 2 C_1 + \ln 4] - a_1(t)$$

Since for $x \to \infty$, the temperature must be finite, hence

$$C_2 = 1/(2\pi t(1 + \sigma)), \quad C_2 = \tau_0/t, \quad \tau_0 = 1/(2\pi(1 + \sigma))$$

Condition (2.14) is the boundary condition for solving the problem in the outer region as $X \to 0$. It follows from (2.4) and (2.6) that solutions in the outer region must satisfy the following equations and boundary conditions:

$$\partial v_1/\partial t = \partial^2 v_1/\partial X^2 \quad (2.15)$$

$$v_1(X \to 0, t) = f(t), \quad v_1(\infty, t) = v_1(X, 0) = 0$$

$$\partial Y_0/\partial t = L^{-1} \partial^2 Y_0/\partial X^2 \quad (2.16)$$

$$Y_0(X \to 0, t) = y_0(t), \quad Y_0(\infty, t) = Y_0(X, 0) = 0$$

The solution of problem (2.15), (2.16) is of the form

$$v_1(X, t) = \frac{X}{2\sqrt{\pi}} \int_0^t f'(t') \frac{\exp[-X^2/(4(t - t'))]}{(t - t')^{3/2}} dt' \quad (2.17)$$

$$Y_0(X, t) = \frac{X L^{1/2}}{2\sqrt{\pi}} \int_0^t y_0(t') \frac{\exp[-X^2/(4(t - t'))]}{(t - t')^{3/2}} dt' \quad (2.18)$$

For $X \to 0$ from (2.18) we have

$$Y_0(X,t) = y_0(t) - \frac{X\sqrt{L}}{\sqrt{\pi}}\frac{d}{dt}\int_0^t \frac{y_0(t')}{\sqrt{t-t'}}dt' + O(X) = \tag{2.19}$$

$$y_0(t) - \frac{x}{\beta}\sqrt{\frac{L}{\pi}}\frac{d}{dt}\int_0^t \frac{y_0(t')}{\sqrt{t-t'}}dt' + O(\beta^{-1})$$

Formula (2.19) makes it possible to obtain the asymptotic expression for $y_1(x, t)$ which is the second term of asymptotic expansion for concentration in the inner region. From (2.4), (2.5) we obtain

$$L^{-1}\partial^2 y_1 / \partial x^2 - \gamma \partial^2 u_1 / \partial x^2 = 0, \quad (\partial y_1 / \partial x)_{x=0} = 0$$

which is accurate to terms β^{-1}. After integration we have

$$L^{-1}\frac{\partial y_1}{\partial x} - \gamma\frac{\partial u_1}{\partial x} = C_3(t), \quad \left(\frac{\partial y_1}{\partial x}\right)_{x=0} = 0; \quad C_3(t) = -\gamma\left(\frac{\partial u_1}{\partial x}\right)_{x=0}$$

consequently,

$$\frac{\partial y_1}{\partial x} = L\gamma\left[\frac{\partial u_1}{\partial x} - \left(\frac{\partial u_1}{\partial x}\right)_{x=0}\right] \tag{2.20}$$

From Eq. (2.19) we obtain the asymptotic expression for $y_1(x \to \infty, t)$

$$y_1 \to -x\sqrt{\frac{L}{\pi}}\frac{\partial}{\partial t}\int_0^t \frac{y_0(t')}{\sqrt{t-t'}}dt' \tag{2.21}$$

We pass in Eq. (2.20) obtained when solving the inner problem, to the outer limit $x \to \infty$. From (2.12), (2.22), and (2.23) we have (*)

$$\partial y_1 / \partial x = -L\gamma(\partial u_1/\partial x)_{x=0} \tag{2.22}$$

and from (2.10)

$$\left(\frac{\partial u_1}{\partial x}\right)_{x=0} = \frac{1}{\pi}\left\{\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{\tau_0}}\left[\frac{\tau_0}{t} - (1-y_0)^n \exp(a_1/(1+\sigma))\right]^{1/2}\right\}$$

Formula (2.22) in dimensionless variables is of the form

$$\frac{d}{d\tau}\int_0^\tau \frac{y_0(\tau')}{\sqrt{\tau-\tau'}}d\tau' = \varepsilon\left[\tau^{-1/2} - G_n(\tau)\right] \tag{2.23}$$

$$G_n(\tau) = [1/\tau - (1-y_0)^n e^{-z}]^{-1/2}$$

$$a_1 = -z(1+\sigma), \quad \tau = t/\tau_0, \quad \varepsilon = \gamma\sqrt{L}$$

The equation for the heater temperature variation is of the form

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*) Editor's Note. There is an obvious error in the Russian text in the numbers of equations (Eqs. (2.12), (2.22), and (2.23)) referred to in this sentence. Attention of the Russian Editor of PMM has been drawn to this. A correction will be issued as soon as received from him.

$$dz/d\tau = \delta G_n(\tau), \quad \delta = \alpha\beta(1+\sigma)^{-1}(\tau_0/\pi)^{1/2} \tag{2.24}$$

Thus the approximate analysis of problem (2.4) using the method of joining asymptotic expansions yields the system of Eqs. (2.23) and (2.24) for the time of ignition, concentration distribution in the gas and the igniting body temperature.

Equations (2.23) and (2.24) are valid in the interval $0 \leqslant \tau \leqslant \tau_{ign}$ (τ_{ign} is the dimensionless ignition time).

Having determined $y_0(t)$ and $z(t)$ we obtain from formulas (2.10), (2.17), (2.18) $u_1(x, t)$, $v_1(X, t)$ and $Y_0(X, t)$, i.e. the total solution of the problem in the first approximation from the instant at which the heat source begins to operate up to the instant of ignition.

Equations (2.23) and (2.24) show the ignition time depends on three dimensionless parameters δ, ε, and n, which considerably simplifies the problem in comparison with its original formulation by (1.15) and (1.20) which comprises six dimensionless combinations of L, α, β, n, γ, and σ.

The particular case of $\delta = 0$ in which Eqs.(2.23) and (2.24) define the igniting of gas by a heated plate maintained at constant temperature was considered in [8]; for $\varepsilon = 0$ these equations relate to the problem of igniting gas by a body of finite heat content without allowance for the reagent burn-up [6].

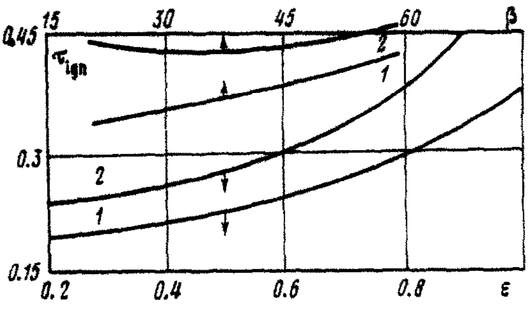

Fig. 1

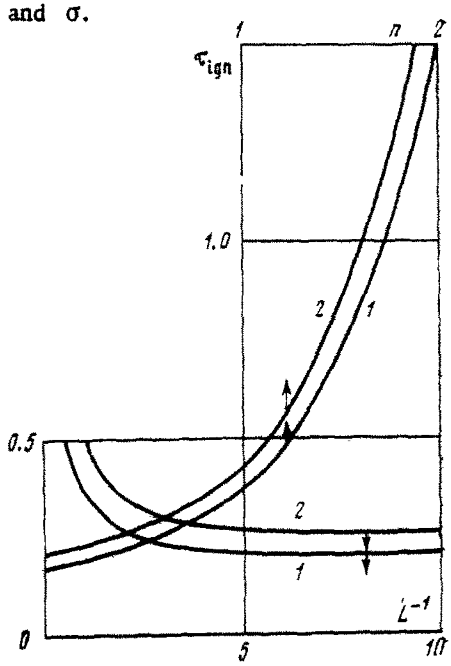

Fig. 2

Equations (2.23) and (2.24) were solved by numerical methods. The dependence of τ_{ign} on parameters ε, n, and δ obtained by that method is shown in Fig. 1—3. The lower curves *1* and *2* in Fig. 1 correspond to $\delta = 0.088$ and 0.77, respectively, and show that with increasing ε the ignition time increases. Physically this is related to the increase of burn-up with increasing ε; since the reaction rate is determined by the law $(1 - y_0)^n \exp[-E/(RT_2)]$, the temperature increase is slowed down with increasing burn-up and the ignition time lengthens.

The upper curves *1* and *2* which in Fig. 2 correspond to $\beta = 20$ and 30, respectively, show that with increase of the reaction order the ignition time sharply increases, which is also related to the increase of burn-up.

The lower curves *1* and *2* which in Fig. 2 correspond to $\beta = 20$ and $\beta = 80$, respectively, show the behavior of numerical solutions of system (2.23), (2.24) of the ignition curve in dependence of the Lewis number $L = \lambda/(D\rho c)$ for two values of β. The characteristic values of L for gases are of order unity.

With decreasing L the quantity τ_{ign} diminishes, which is related to that in this case the diffusion influx of fresh fuel increases and the effect of burn-up is decreased. Since the reaction rate obeys the lay $\Phi \sim \exp[-E/(RT_2)]$, hence the temperature increase is more rapid and the ignition time is lengthened.

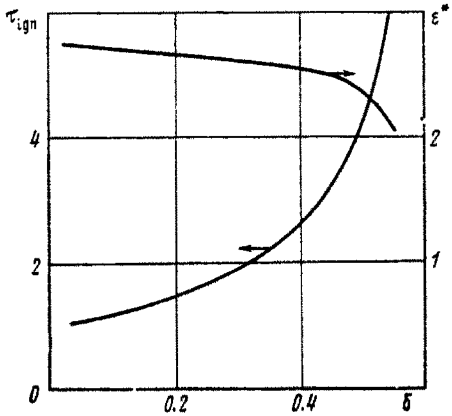

Fig. 3

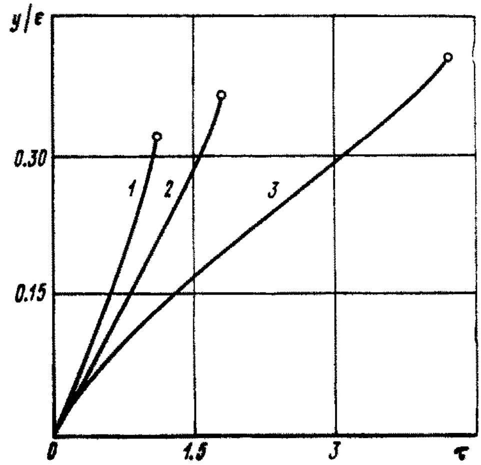

Fig. 4

All of the above examples dealt with cases in which ignition always takes place. However, situations are possible in which the outflow from the heat source exceeds the heat release rate dependent on chemical transformation, and ignition does not occur. Let us consider such case, assuming for simplicity that the reaction is of zero order so that for $0 \leqslant y \leqslant 1$ the chemical reaction rate is $k \exp[-E/(RT_2)]$ and vanishes for $y > 1$.

The dependence of τ_{ign} on δ obtained by numerical integration of Eqs. (2.23) and (2.24) with $n = 0$ appears in Fig. 3 which shows that the ignition time lengthens with increasing δ. There exists a δ^* such that for $\delta > \delta^*$ ignition does not occur. Note that all results must be taken in the asymptotic sense. Since for $\delta > \delta^*$ the ignition time is considerable in comparison with unity and the asymptotic investigation covers times of the order of unity relative to β, hence in the considered approximation no ignition occurs when $\delta > \delta^*$. The critical value $\delta = \delta^*$ determined by numerical integration is $\delta^* = 0.57$.

For fairly large ε a complete burn-up may occur prior to ignition. Variation of the concentration fields within the time up to the ignition instant is shown in Fig. 4 for several δ, where curves *1* — *3* correspond to $\delta = 0.1$, 0.3, and 0.5, respectively. There exists an $\varepsilon = \varepsilon^*$ for which y becomes equal unity before ignition takes place. The dependence of ε^* on δ is shown in Fig. 3. For ε lying above ε^* total burn-up occurs before ignition, while for $\varepsilon < \varepsilon^*$ ignition takes place prior to the burn-up. For ε lying on the curve ignition and total burn-up occur simultaneously.

The accuracy of asymptotic methods in their application to problems of ignition was tested by solving Eqs. (1.3) numerically. The method of "calculation with re-calculation" [12] was used. Results of calculations by approximate analytical methods are shown in Fig. 5 for $n = 1$ and $\alpha = 10^{-2}$ and compared with those derived by numerical methods which appear in Fig. 1, where the upper curves *1* and *2* correspond to the approximate analytical and numerical methods, respectively; in both figures the curves show the dependence of ignition time on β.

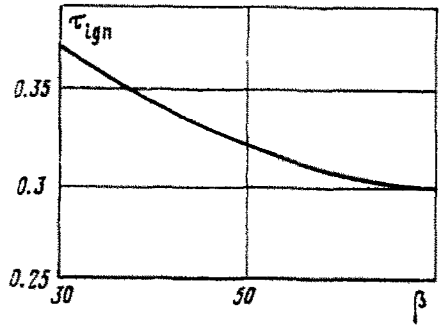

Fig. 5

As expected, the accuracy of calculations increases with the increase of β. The difference between the approximate analytical and exact numerical calculations for $\beta = 20$ is about 20% which with increasing β diminishes to 5 – 10%. Note that only the principal terms of expansion were determined here. When subsequent expansion terms are taken into account, the disparity between data obtained by the two methods diminishes.

The obtained good agreement between the results of the two methods indicates that the use of the method of joining asymptotic expansions is promising also for other problems of combustion.

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