HETEROGENEOUS IGNITION AND EXTINGUISHING OF A PARTICLE WITH CONSIDERATION OF RADIANT HEAT EXCHANGE

V. V. Kalinchak, S. G. Orlovskaya, and A. I. Kalinchak

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The effect of radiation on the critical ignition and extinction parameters of a coal particle in air is studied.

Consideration of thermal losses due to radiation produces new qualitative dependences for the limits of heterogeneous particle ignition [1, 2]. At a wall temperature less than the gas temperature a minimum occurs in the ignition temperature curve, the nature of which is related to heat loss by radiation [2].

Analysis of heterogeneous combustion and self-extinction of a coal particle in air has shown that heat losses by radiation lead to a significant narrowing of combustion temperatures and increase in the diameter of a self-extinguishing particle [3-5]. In addition, the effect of radiation on parameters of forced and spontaneous extinction have not been studied sufficiently. The effect of radiation on degeneration of critical ignition and extinction conditions remains practically unstudied.

The present study will analyze heterogeneous ignition and extinction using the example of a coal particle, on the surface of which a single reaction occurs: $C + O_2 \rightarrow CO_2$. Analytical expressions will be derived for the critical diameters for ignition, forced, and spontaneous extinction, with consideration of radiant heat exchange. The effect of radiation on the dependence of combustion temperature on particle diameter will be considered. Degeneration of critical ignition and extinction conditions in the range of large and small particles will be examined.

The critical ignition and extinction parameters and combustion temperature can be found by solving the equations of nonsteady heat-mass transport and analysis of the stability of steady-state heat-mass transport regimes. For $Bi \ll 1$ the equations of nonsteady heat-mass transport and kinetics of a heterogeneous reaction have the form [3]

$$\frac{1}{6} c_1 \rho_1 \delta \frac{dT_1}{dt} = Q_c - Q_t, \quad T_1(t=0) = T_{1in};$$

$$\frac{d\delta}{dt} = -\frac{2\Omega Q_c}{q\rho_1}, \quad \delta(t=0) = \delta_{in}, \tag{1}$$

where

$$Q_c = q n_{ox} \rho_2 \left(\frac{1}{k} + \frac{1}{\beta} \right)^{-1}, \quad k = k_0 \exp\left(-\frac{E}{RT_1} \right), \tag{2}$$

$$\beta = D\,\mathrm{Nu}/\delta, \quad D = D_0 (T_1/T_0)^{n+1}, \quad \rho_2 = \rho_{20} (T_0/T_1), \tag{3}$$

$$Q_T = Q_{mc} + Q_r, \quad Q_{mc} = \alpha (T_1 - T_2), \quad \alpha = \lambda_2 \mathrm{Nu}/\delta, \quad \lambda_2 = D c_2 \rho_2, \tag{4}$$

$$Q_r = \varepsilon\sigma (T_1^4 - T_w^4). \tag{5}$$

For air the exponent n = 0.75. Ignition, combustion, and extinction characteristics can be found from the functions $T_1(t)$, $dT_1/dt(t)$, $\delta(t)$. Completion of exit to the high-temperature regime (combustion) is determined by the induction period, i.e., the time over which $dT_1/dt > 0$ takes on its maximum value, $d^2T_1/dt^2 = 0$, $d^3T_1/dt^3 < 0$ [1, 3]. The reaction rate constant then becomes comparable to the mass-exchange coefficient. After reaching the maxi-

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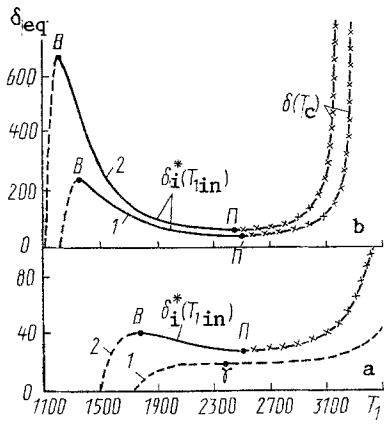

Fig. 1

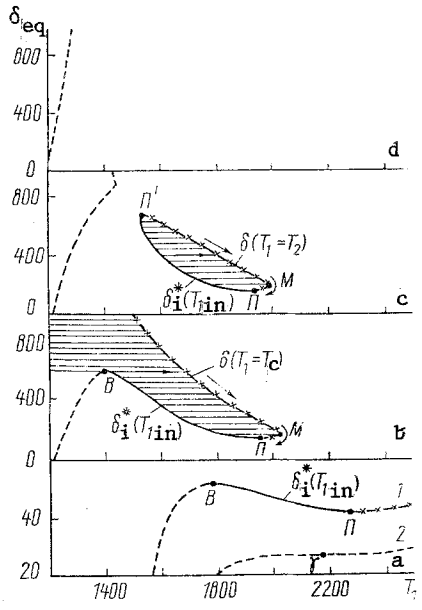

Fig. 2

Fig. 1. Equilibrium particle diameter vs particle temperature without consideration of radiant heat loss ($\varepsilon = 0$): a) 1, $T_2 = 1735$; 2, 1500; b) 1, 1210; 2, 1100. δ, μm; T, K.

Fig. 2. Evolution of $\delta_{eq}(T_1)$ curves with consideration of radiant heat loss ($\varepsilon = 0.78$) at $T_w = T_2$: a) 1, 1500; 2, $T_2 = T_\gamma = 1650$; b) 1220; c) 1210; d) $T_2 = 1190$.

mum value the combustion temperature decreases and when the particle diameter attains the critical value spontaneous extinction occurs [3-5]. The spontaneous extinction diameter δ_e can be determined from the curve $\delta(t)$ for the moment in time at which $dT_1/dt < 0$, $d^2T_1/dt^2 = 0$ and $d^3T_1/dt^3 > 0$.

The diameters for forced and spontaneous extinction can be found by analyzing the stability of the heterogeneous reaction thermal regime $dT_1/dt = 0$, i.e., $Q_c = Q_t$. Substituting Eqs. (2)-(5) in the condition $Q_c = Q_t$, we obtain an expression for the equilibrium particle diameter as a function of temperature in the explicit form

$$\delta_{eq} = \frac{\lambda_{20}\,\mathrm{Nu}}{\alpha_{eq}} = \frac{D_0\,\mathrm{Nu}}{\beta_{eq}} = \frac{\lambda_2 (T_1 - T_2)\,\mathrm{Nu}}{(A \pm \sqrt{A^2 - B})\, q n_{ox}\, \rho_2 k_0} \exp \frac{E}{RT_1}, \tag{6}$$

where

$$A = \frac{1}{2}\left[1 - \frac{c_2 (T_1 - T_2)}{q n_{ox}} - \frac{\varepsilon\sigma (T_1^4 - T_w^4)}{q n_{ox}\, \rho_2 k}\right],$$

$$B = \frac{\varepsilon\sigma (T_1^4 - T_w^4)\, c_2 (T_1 - T_2)}{\rho_2 k\, (q n_{ox})^2}. \tag{7}$$

If we take the plus sign of the root in Eq. (6), then at $\varepsilon = 0$ we obtain the well-known expression presented in [4]:

$$\delta_p = \frac{\lambda_2 (T_1 - T_2)}{q n_{ox} \rho_2 k_0}\left[1 - \frac{c_2 (T_1 - T_2)}{q n_{ox}}\right]^{-1} \exp \frac{E}{RT_1}. \tag{8}$$

The minus sign in Eq. (6) defines qualitative effects related to heat loss by radiation, since at $\varepsilon = 0$ we obtain $\delta_r = \infty$.

Analysis of $\delta_{eq}(T_1)$ at $\varepsilon = 0$ and $\varepsilon = 0.78$ together with the expressions $Q_c(T_1)$ and $Q_t(T_1)$ for various gas temperatures permits clarification of the effect of radiation on the critical ignition and extinction diameters, the dependence of critical ignition diameter on initial particle temperature $\delta_i^*(T_{1in})$ and the dependence of combustion temperature on particle diameter $T_c(\delta)$. For the case $\varepsilon = 0$ (Fig. 1) the curve $\delta_{eq}(T_1)$ has two extrema, corresponding to

tangency of the curves $Q_c(T_1)$ and $Q_t(T_1)$, i.e., the condition $\partial Q_c/\partial T_1 = \partial Q_t/\partial T_1$. The maximum of $\delta_{eq}(T_1)$ for T_{1i} defines the ignition diameter δ_i, the minimum at T_{1e} corresponding to the spontaneous extinction diameter δ_e. The branch of $\delta_{eq}(T_1)$ joining the extrema defines the dependence of critical ignition diameter on initial particle temperature $\delta_i^*(T_{1in})$. On Semenov diagrams this corresponds to intersection of the curves $Q_c(T_1)$ and $Q_t(T_1)$ at a point for which $\partial Q_c/\partial T_1 > \partial Q_t/\partial T_1$. The dashed line $\delta_{eq}(T_1)$ defines the low-temperature oxidation regime, while the high-temperature regime of combustion is defined by the branch $\delta(T_c)$. With decrease in gas temperature δ_i and δ_e increase monotonically, as does the ignition diameter, but to a greater degree (Fig. 1b, curves 2 and 1). With increase in T_2 the quantities δ_i and δ_e approach each other and degenerate at $T_2 = T_{2\gamma}$ at the inflection point (point γ on Fig. 1a, curve 1).

When radiant heat loss is considered ($\varepsilon = 0.78$, $T_w = T_2$) in the high gas temperature region (Fig. 2a, curves 1 and 2), just as in the case $\varepsilon = 0$ at $T_2 = T_{2\gamma}$ the extrema corresponding to ignition and extinction degenerate at the inflection point (point γ in Fig. 2a, curve 2). With decrease in gas temperature the evolution of the $\delta_{eq}(T_1)$ curves occurs in a manner qualitatively different from the case $\varepsilon = 0$. Decrease in gas temperature below some value $T_{2\gamma'}$ (in the given case $T_{2\gamma'} = 1212$ K) leads to degeneration of the maximum accompanying ignition (point Π') (Fig. 2b, c). The combustion branch $\delta(T_c)$ joins with the ignition branch, defining the dependence of critical ignition diameter on initial particle temperature $\delta_i^*(T_{1in})$ at the point Π'. Further decrease in gas temperature produces only a low-temperature oxidation regime – the dashed line $\delta_{eq}(T_1)$ (Fig.2d), i.e., at $\varepsilon \neq 0$ there exists a limiting gas temperature (which we will call T_{2c}), below which the high-temperature heterogeneous reaction regime cannot be achieved by change in particle diameter or initial temperature.

As is evident from Figs. 1, 2, radiant heat loss reduces the effect of initial particle temperature on critical ignition diameter. In analytical form $\delta_i^*(T_{1in})$ is described by Eqs. (6)-(8), in which we set $T_1 = T_{1in}$.

Consideration of radiant heat loss leads to new qualitative and quantitative principles involving the dependence of combustion temperature on particle diameter. The dashed region of Fig. 2 determines the parameters for which the transition to the high-temperature combustion branch $\delta(T_c)$ (denoted by horizontal arrow) occurs. As a result of combustion the particle diameter decreases, the combustion temperature increases, and passes through a maximum (the point M). In Fig. 2b, c the change in T_c with decrease in particle diameter is shown by an arrow along the curve $\delta(T_c)$. For further decrease in diameter to the critical value δ_e the combustion temperature decreases to T_{1e}. The maximum combustion temperature and corresponding diameter can be found from Eqs. (6), (7), and the condition $A^2 = B$:

$$T_{cm} = T_2 + \frac{qn_{ox}}{c_2}\left[1 - \sqrt{\frac{s\sigma(T_{cm}^4 - T_w^4)}{k_0 qn_{ox}\rho_2}}\exp\frac{E}{2RT_{cm}}\right]^2,$$

$$\delta_m = \frac{D\,\mathrm{Nu}}{k_0}\left[\sqrt{\frac{qn_{ox}}{c_2(T_{cm} - T_2)}} - 1\right]^{-1}\exp\frac{E}{RT_{cm}}. \qquad (9)$$

At $\varepsilon = 0$ we obtain the well-known expression for the heterogeneous combustion temperature of a particle in the diffusion regime. For $\delta > \delta_m$ the combustion temperature is determined from Eq. (6) with a minus sign before the root

$$\delta = \frac{\lambda_2(T_c - T_2)\,\mathrm{Nu}}{(A_c - \sqrt{A_c^2 - B_c})k_0 qn_{ox}\rho_2}\exp\frac{E}{RT_c},$$

where A_c and B_c can be found from Eq. (7) at $T_1 = T_c$. Calculations of T_{cm}, δ_m, the dependence of T_c on δ with the expressions obtained and the nonsteady model of Eqs. (1)-(5) were found to be in good agreement and are confirmed by the experimental data of [6].

To determine the dependence of particle critical diameters and temperatures which determine ignition and extinction upon gas temperature we use the condition of instability of the steady-state heat-mass exchange regime: $\partial Q_c/\partial T_1 = \partial Q_t/\partial T_1$. Considering the temperature dependence of the thermal conductivity coefficient and gas density, we obtain the expression

$$qn_{ox}\rho_2\left(\frac{1}{k}+\frac{1}{\beta}\right)^{-1}\left\{\left(\frac{1}{k}+\frac{1}{\beta}\right)^{-1}\left[\frac{E}{RT_1^2k}+\frac{(n+1)}{T_1\beta}\right]-\frac{1}{T_1}\right\}=\alpha\left[1+\frac{(T_1-T_2)}{T_1}n\right]+4\varepsilon\sigma T_1^3, \quad (10)$$

where

$$\alpha = c_2\rho_2\beta = qn_{0x}\rho_2 k\,(A \pm \sqrt{A^2-B})/(T_1-T_2), \quad (11)$$

which defines the dependence of critical particle temperature on gas temperature with consideration of radiant heat loss. For the case $\varepsilon = 0$ and neglecting the effect of temperature on thermophysical properties this dependence has been obtained in explicit form [4]. For a plus sign before the root in Eq. (11), Eq. (10) has two solutions. The lower value $T_{1cr} = T_{1i}$ corresponds to ignition, the higher $T_{1cr} = T_{1e}$, to particle extinction. Substituting T_{1i} in Eq. (7), we obtain the dependence of critical ignition diameter δ_i on T_{1i} on $T_{1i}(T_2)$:

$$\delta_{cr} = \delta_i = \frac{\lambda_2(T_{1i}-T_2)\,\mathrm{Nu}}{(A_i+\sqrt{A_i^2-B_i})\,qn_{ox}\rho_2 k_0}\exp\frac{E}{RT_{1i}}, \quad (12)$$

where A_i and B_i are defined by Eq. (7) at $T_1 = T_{1i}$. For spontaneous and constrained extinction of a particle we have the diameters

$$\delta_{cr} = \delta_e = \frac{\lambda_2(T_{1e}-T_2)\,\mathrm{Nu}}{(A_e+\sqrt{A_e^2-B_e})\,qn_{ox}\rho_2 k_0}\exp\frac{E}{RT_{1e}}, \quad (13)$$

where A_e and B_e are defined by Eq. (7) at $T_1 = T_{1e}$. Figures 3 and 4 show the dependence of particle critical diameters and temperatures on gas temperature at $\varepsilon = 0$ and $\varepsilon = 0.78$, $T_w = T_2$, $T_w < T_2$.

For the temperature interval $T_{2c} < T_2 < T_{2\gamma}'$ we obtain the dependence of the diameter for forced extinction on gas temperature if in Eq. (11) we take the minus sign before the root:

$$\delta_{cr} = \delta_{e'} = \frac{\lambda_2(T_{1e'}-T_2)\,\mathrm{Nu}}{(A_{e'}-\sqrt{A_{e'}^2-B_{e'}})\,qn_{ox}\rho_2 k_0}\exp\frac{E}{RT_{1e'}},$$

where A_e' and B_e' are defined by Eq. (7) at $T_1 = T_{1e}'$.

The dependences of particle critical diameter and ignition and extinction temperature on gas temperature in the presence of radiation (Fig. 3, curves 2 and Fig. 4) differ qualitatively from those calculated without consideration of radiation (Fig. 3, curves 1). For $\varepsilon = 0$ decrease in gas temperature leads to monotonic increase in δ_i and δ_e, with δ_i increasing to a greater extent than δ_e. For $\varepsilon = 0.78$ and $T_w = T_2$ (Fig. 3, curves 2) as T_2 decreases δ_i and δ_e, T_{1i} and T_{1e} approach each other and the critical conditions degenerate at $T_2 = T_{2\gamma}'$.

In the region of high gas temperatures (small particle dimensions) at $\varepsilon = 0$ and $\varepsilon = 0.78$ the behavior of the critical temperature and diameter is qualitatively the same. Degeneration of critical ignition and extinction conditions (points γ, Figs. 3 and 4) is determined essentially by conductive heat losses. However, with consideration of radiant heat loss δ_i and δ_e are larger, and the critical temperatures T_{1i}, T_{1e}, $T_{2\gamma}$ are lower than for $\varepsilon = 0$.

For the case where the wall temperature is less than the gas temperature the behavior of the curves $\delta_i(T_2)$ and $\delta_e(T_2)$, $T_{1i}(T_2)$ and $T_{1e}(T_2)$ in the large particle diameter range changes qualitatively (Fig. 4). Increase in gas temperature, beginning at some limiting T_{2c}' (point C' in Fig. 4) leads to both growth and reduction in particle critical diameters and temperatures for ignition. With increase in T_2, beginning at some temperature T_{2c} (point C in Fig. 4), the constrained extinction diameter δ_e' increases, while T_{1e}' decreases and the diameter δ_e decreases, and T_{1e} increases.

In the temperature range $T_{2c} < T_2 < T_{2c}'$ a particle can be ignited by change in diameter and initial temperature within the ranges $\delta_e < \delta < \delta_e'$ and $T_{1e} < T_{1in} < T_{1e}'$.

To find the limiting temperatures T_{2c} and T_{2c}' we consider that those values determine the position of the minimum on the curve of critical gas temperature vs particle diameter. Using the Semenov conditions $Q_c = Q_t$ and $\partial Q_c/\partial T_1 = \partial Q_t/\partial T_1$, and the condition of a minimum on the curve $T_{2cr}(\delta)$, neglecting the temperature dependence of λ_2 and ρ_2, we obtain a system of equations defining the limiting particle and gas temperatures and the corresponding diameters as a function of oxidizer concentration and wall temperature:

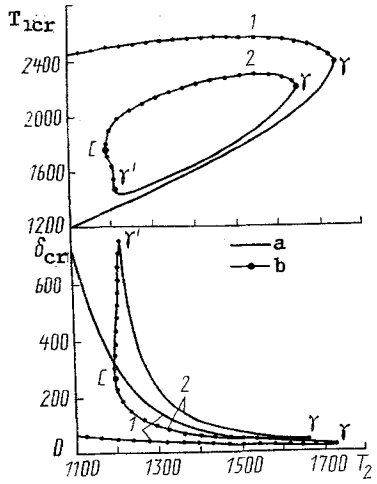

Fig. 3

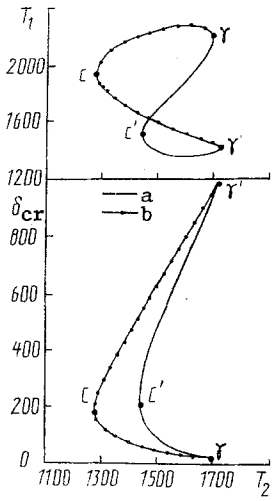

Fig. 4

Fig. 3. Effect of radiant heat loss on dependence of critical particle diameter and temperature upon gas temperature: a) $\delta_i(T_2)$, $T_{1i}(T_2)$; b) $\delta_e(T_2)$, $T_{1e}(T_2)$; 1, $\varepsilon = 0$; 2, 0.78.

Fig. 4. Particle critical diameter and temperature vs gas temperature at $T_w = 500$ and $\varepsilon = 0.78$; a) $\delta_i(T_2)$, $T_{1i}(T_2)$; b) $\delta_e(T_2)$, $T_{1e}(T_2)$.

$$\frac{\varepsilon\sigma T_1^2 (E/R)}{c_2\rho_2 k}\left(1-\frac{T_w^4}{T_1^4}-\frac{4RT_1}{E}\right)\left(\sqrt{\frac{qn_{ox}\rho_2 k}{\varepsilon\sigma(T_1^4-T_w^4)}}-1\right)=1, \tag{14}$$

$$\frac{\varepsilon\sigma T_1^2 (E/R)\delta}{\lambda_2 \mathrm{Nu}}\left(1-\frac{T_w^4}{T_1^4}-\frac{4RT_1}{E}\right)=1, \tag{15}$$

$$T_2 = T_1 + \frac{\varepsilon\sigma\delta}{\lambda_2 \mathrm{Nu}}(T_1^4-T_w^4)-\frac{qn_{ox}\rho_2\delta}{\lambda_2 \mathrm{Nu}}\left(\frac{1}{k}+\frac{\delta}{D\,\mathrm{Nu}}\right)^{-1}. \tag{16}$$

For the kinetic region of heterogeneous reaction development, neglecting $\delta/D\mathrm{Nu}$ in comparison to $1/k$ in Eq. (16) it is simple to obtain the condition for a minimum on the curve $T_{2cr}(\delta)$:

$$T_{2c'} = T_2 = T_1 \quad \text{and} \quad K_R\left(1-\frac{T_w^4}{T_2^4}-\frac{4RT_2}{E}\right)=1, \tag{17}$$

where K_R is the radiant heat exchange criterion:

$$K_R = \varepsilon\sigma T_2^2 E/R\lambda_2 \mathrm{Nu}.$$

Equation (15) is more precise than the condition $K_R(1 - T_w^4/T_2^4) = 1$ obtained in [2].

By using system (14)-(16) it can easily be proved that an increase in oxidizer concentration leads to decrease in limiting temperature to a greater extent than does increase in wall temperature.

The degeneration parameters can be found from the condition $\partial^2\delta_{eq}/\partial T_1^2 = 0$ for $T_2 = \text{const}$ or $\partial^2 T_{eq}/\partial T_1^2 = 0$ at $\delta = \text{const}$. This is identical to the equation

$$\partial^2 Q_c/\partial T_1^2 = \partial^2 Q_t/\partial T_1^2, \tag{18}$$

which is solved simultaneously with the Semenov conditions

$$Q_c = Q_t \quad \partial Q_c/\partial T_1 = \partial Q_t/\partial T_1. \tag{19}$$

Degeneration parameters can be obtained in explicit form only for the case $\varepsilon = 0$ with neglect of the temperature dependence of λ_2 and ρ_2 [5]. Solution of the transcendental system (18), (19) shows that in the region of coarse particles the degeneration diameter $\delta_{Y'}$ in-

creases with increase in oxidizer concentration. Thus, increase in n_{ox} from 0.23 to 0.35 produces growth from $\delta_{\gamma}' = 730$ to $\delta_{\gamma}' = 2200$ μm. The degeneration diameter δ_{γ}' increases with decrease in wall temperature.

Thus, it has been shown that consideration of radiant heat loss leads to qualitatively and quantitatively new principles in heterogeneous ignition, extinction, combustion, and degeneration conditions for coarse particles.

NOTATION

Q_c, surface heat liberation power due to chemical reaction, J/(m²·sec); Q_t, net thermal flux density of molecular convective Q_{mc} and radiant Q_r sources, J/(m²·sec); δ, particle diameter, m; t, time, sec; T_1, T_2, T_w, temperature of particle, gas, and chamber wall, K; ρ_1, ρ_2, density of particle and gaseous medium, kg/m³; c_1, c_2, specific heat of particle and gas, J/(kg·K); Ω, stoichiometric coefficient; Nu, Nusselt number; λ_2, D, gas thermal conductivity and diffusion coefficients, W/(m·K), m²·sec; q, thermal effect of chemical reaction, J/kg; n_{ox}, relative mass concentration of oxidizer in gas mixture; E, activation energy, J/mol; R, universal gas constant J/(mol·K); k_0, pre-exponential factor, m/sec; ρ_{20}, λ_{20}, D_0, gas density, thermal conductivity and diffusion coefficients at temperature T_0; ε, emissivity; σ, Stefan–Boltzmann constant, W/(m²·K⁴); α, β, heat and mass transport coefficients, W/(m²·K), m/sec. Subscripts: 1, particle; 2, gas; i, ignition; e, extinction; eq, equilibrium; cr, critical; c, combustion; m, maximum; γ, degenerate; c, limiting.

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DEFLAGRATION OF TITANIUM IN OXYGEN FOR VARIOUS RATES OF EXPOSURE OF JUVENILE METAL SURFACE

V. I. Bolobov, K. M. Makarov, and A. A. Prokof'ev

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We present the results of an experimental study of the process of deflagration of titanium VT1-0 samples during fracture in oxygen at various pressures. We propose an empirical equation, which describes the critical deflagration pressure of the samples as a function of the exposure rate of juvenile metal surface.

It is known [1-5] that a necessary condition for deflagration of titanium constructions in oxygen-containing media at normal temperatures is the emergence of juvenile (freshly exposed) metal surface. At the same time, the question of the rate at which juvenile surface must be formed for this process to occur has not been sufficiently studied. So, for example, [5] merely points out that titanium alloys deflagrate only when fracture of the structure takes place "rapidly"; "slowly" developing fracture does not lead to deflagration. Data from [2] indicates that the rate of uniaxial elongation of samples during their failure in oxygen does not significantly influence the critical deflagration pressure P_{cr} of titanium α alloys. (These experiments were carried out in the range of clamp displacements of V = 0.017-2.3 mm/sec). In this case, the value of P_{cr} depends essentially on the geometrical dimensions

State Institute of Applied Chemistry, St. Petersburg.

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