TOWARD A STEADY-STATE THEORY OF HETEROGENEOUS IGNITION AND EXTINCTION OF A PARTICLE IN A HEATED GASEOUS OXIDIZER

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Expressions are obtained for critical diameters of particles limiting the regions of existence of the heterogeneous processes of combustion and extinction.

The transition from combustion to extinction of a particle reacting with a gas by the rule $\nu_1 A_1$(solid) + $\nu_2 A_2$(gas) → $\nu_3 A_3$(gas) in a heated oxidizer is related to an increase in heat liberation caused by reduction in particle size [1].

Analysis of ignition and extinction based on Frank-Kamenetskii's concepts [2, 3] and neglect of the effect of temperature on the transport coefficients and gas density reduces the accuracy of the results for the critical extinction condition and the degeneracy criterion.

The present study will analyze ignition and extinction of a particle without use of the Frank-Kamenetskii transforms with and without consideration of the effect of temperature on thermophysical properties.

Semenov's conditions

$$Q_c = Q_1, \quad \frac{dQ_c}{dT} = \frac{dQ_1}{dT}, \tag{1}$$

where

$$Q_c = qn_{ox_2}\rho_{2*}\frac{T_*}{T_1}\left[\frac{\exp(E/RT_1)}{k_0} + \frac{dT_*^{n+1}}{\mathrm{Nu}\,D_* T_1^{n+1}}\right]^{-1}, \tag{2}$$

$$Q_1 = \mathrm{Nu}\frac{\bar{\lambda}_{2*}}{d}\left(\frac{T_1}{T_*}\right)^n (T_1 - T_2), \tag{3}$$

characterize the critical diameters corresponding to ignition and extinction of a particle in a heated oxidizer.

Figure 1 shows calculated curves for anthracite coal, reacting with atmospheric oxygen by the reaction C + O_2 → CO_2. Physical properties are taken from [2]. The calculations were performed for an oxidizer concentration in the air n_{ox_2} = 0.23 and pressure P = 10^5 Pa, exponent n = 0.75, Nu = 2.

For a large diameter particle with d = 180 μm Q_c and Q_1 intersect, giving a stable point corresponding to combustion. With decrease in particle radius the Q_c and Q_1 curves change (shown by the arrow in Fig. 1), and finally at d_e = 43.4 μm they become tangent, and the particle extinguishes.

The upper portion of Fig. 1 illustrates tangency of Q_c and Q_1 at a critical particle diameter of d_i = 127.8 μm.

Thus, at T_2 = 1300 K all particles with d > d_i = 127.8 μm ignite, burn and extinguish upon reaching d_e = 43.4 μm.

Without considering the dependence of ρ, D, λ on temperature (n = 0) we will find the critical temperature and diameter of a particle corresponding to its ignition and extinction. For simplicity we assume D = $\lambda_2/c_2\rho_2$.

Substituting Eqs. (2), (3) in Eq. (1) we obtain

$$qn_{ox_2}\rho_2\left[\frac{\exp(E/RT_1)}{k_0} + \frac{dc_2\rho_2}{\lambda_2\,\mathrm{Nu}}\right]^{-1} = \mathrm{Nu}\,\frac{\bar{\lambda}_2}{d}(T_1 - T_2), \tag{4}$$

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$$qn_{ox2}\rho_2\left[\frac{\exp(E/RT_1)}{k_0}+\frac{dc_2\rho_2}{\lambda_2 \mathrm{Nu}}\right]^{-2}\frac{E\exp(E/RT_1)}{RT_1^2k_0}=\mathrm{Nu}\frac{\lambda_2}{d} \tag{5}$$

– a system of equations in T_1 and T_2. Using Eq. (4) to express the particle diameter

$$d=\mathrm{Nu}\frac{\lambda_2c_2(T_1-T_2)}{c_2\rho_2k_0[qn_{ox2}-c_2(T_1-T_2)]}\exp\frac{E}{RT_1} \tag{6}$$

and substituting the latter in Eq. (5), we obtain an equation relating T_1 and T_2:

$$(T_1-T_2)^2\left[\frac{qn_{ox2}}{c_2(T_1-T_2)}-1\right]^2-\frac{RT_1^2qn_{ox2}}{Ec_2}\left[\frac{qn_{ox2}}{c_2(T_1-T_2)}-1\right]=0. \tag{7}$$

The first root of Eq. (7)

$$T_1=T_2+\frac{qn_{ox2}}{c_2}$$

yields d = ∞, corresponding to total occurrence of the reaction in the diffusion regime, not a physically realizable situation.

We define two other roots by solution of an equation which follows from Eq. (7):

$$T_1^2\left(1+\frac{Rqn_{ox2}}{Ec_2}\right)-2\left(T_2+\frac{qn_{ox2}}{2c_2}\right)T_1+T_2^2+\frac{qn_{ox2}}{c_2}T_2=0$$

in the form

$$T_{1i}=\left(1+\frac{Rqn_{ox2}}{Ec_2}\right)^{-1}\left[T_2+\frac{qn_{ox2}}{2c_2}(1-\sqrt{\gamma})\right], \tag{8}$$

$$T_{1e}=\left(1+\frac{Rqn_{ox2}}{Ec_2}\right)^{-1}\left[T_2+\frac{qn_{ox2}}{2c_2}(1+\sqrt{\gamma})\right]. \tag{9}$$

Here

$$\gamma=1-\frac{4RT_2}{E}-\frac{4RT_2^2c_2}{Eqn_{ox2}}, \tag{10}$$

where T_{1i} is the particle temperature at which ignition occurs, and T_{1e} is the extinction temperature.

Equations (8)-(10) have meaning only for γ > 0, i.e., at

$$\xi=\frac{qn_{ox2}E}{RT_2^2c_2}>4\left(1+\frac{qn_{ox2}}{c_2T_2}\right),$$

which differs by $qn_{ox2}/c_2T_2 > 1$ from ξ obtained with use of the Frank-Kamenetskii transform [1-3].

Substituting Eqs. (8) and (9) in Eq. (6) we find

$$d_i=\frac{\mathrm{Nu}D(1-\sqrt{\gamma}-2RT_2/E)}{k_0[1+\sqrt{\gamma}+2R(T_2+qn_{ox2}/c_2)/E]}\exp\frac{E(1+qn_{ox2}R/c_2E)}{R[T_2+(qn_{ox2}/2c_2)(1-\sqrt{\gamma})]} \tag{11}$$

– the critical diameter below which a particle will not ignite at a given temperature – and

$$d_e=\frac{\mathrm{Nu}D(1+\sqrt{\gamma}-2RT_2/E)}{k_0[1-\sqrt{\gamma}+2R(T_2+qn_{ox2}/c_2)/E]}\exp\frac{E(1+qn_{ox2}R/c_2E)}{R[T_2+(qn_{ox2}/2c_2)(1+\sqrt{\gamma})]} \tag{12}$$

– the critical diameter at which particle extinction occurs.

It can easily be seen from the expressions for d_i and d_e that

$$\frac{1-\sqrt{\gamma}-2RT_2/E}{1+\sqrt{\gamma}+2R(T_2+qn_{ox2}/c_2)/E}\ll 1,$$

$$\frac{1+\sqrt{\gamma}-2RT_2/E}{1-\sqrt{\gamma}+2R(T_2+qn_{ox2}/c_2)/E}\geqslant 1.$$

Then, correspondingly

$$\frac{k_0d_i}{D\,\mathrm{Nu}}\exp\left(-\frac{E}{RT_{1i}}\right)\ll 1,\qquad \frac{k_0d_e}{D\,\mathrm{Nu}}\exp\left(-\frac{E}{RT_{1e}}\right)\geqslant 1.$$

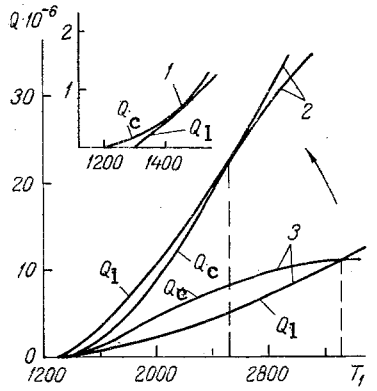

Fig. 1

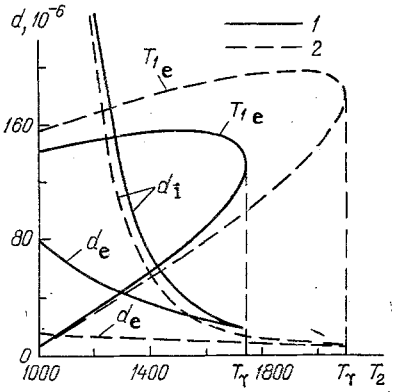

Fig. 2

Fig. 1. Quantities Q_c and Q_1 vs particle temperature T (K) for anthracite at constant air temperature T_2 = 1300 K and various diameters: 1) 127.8 μm; 2) 43.4; 3) 180. Q in W/m^2.

Fig. 2. Critical diameters d_i, d_e (m) and temperatures T_{1i} and T_{1e} (K) vs medium temperature: 1, with consideration of temperature dependence of properties; 2, without such consideration.

Consequently, ignition occurs in the kinetic regime, and extinction in the transitional regime. An approximate analysis will be useful for purposes of comparison with expressions available in the literature. At large activation energies and correspondingly low medium temperatures $4RT_2/E < 1$, $4RT_2^2c_2/Eqn_{ox_2} < 1$, $Rqn_{ox_2}/Ec_2 < 1$. Expanding $\sqrt{\gamma}$ in a series, we obtain

$$T_{1e} - T_2 = \frac{RT_2^2}{E}\left(1 + \frac{qn_{ox_2}R}{Ec_2}\right)^{-1} \approx \frac{RT_2^2}{E}. \tag{13}$$

Then the critical ignition condition

$$\frac{k_0 d_i}{D\,\mathrm{Nu}} \exp\left[-\frac{E}{R(T_2 + RT_2^2/E)}\right] \approx \frac{RT_2^2 c_2}{Eqn_{ox_2}} = \frac{1}{\xi} \tag{14}$$

coincides with that presented in [3], although calculation with Eqs. (13) and (14) yields significant errors as compared to the precise expressions (8), (11), and (10).

In a similar manner we obtain for the extinction temperature and critical condition

$$T_{1e} = T_m - \frac{RT_m^2}{E}\left(1 + \frac{qn_{ox_2}R}{c_2E}\right)^{-1} \approx T_m - \frac{RT_m^2}{E}, \tag{15}$$

where $T_m = T_2 + qn_{ox_2}/c_2$,

$$\frac{k_0 d_e}{D\,\mathrm{Nu}} \exp\left[-\frac{E}{R(T_m - RT_m^2/E)}\right] = \frac{qn_{ox_2}E}{c_2RT_m^2} = \xi\left(\frac{T_2}{T_m}\right)^2, \tag{16}$$

which are more correct than the expressions in [1, 3].

With increase in medium temperature d_i and d_e decrease, while T_{1i} and T_{1e} increase, tending respectively to d_γ and $T_{1\gamma}$ at $T_{2\gamma}$, which is defined from the condition

$$\gamma = 1 - \frac{4RT_{2\gamma}}{E} - \frac{4RT_{2\gamma}^2 c_2}{Eqn_{ox_2}} = 0$$

in the form

$$T_{2\gamma} = \frac{qn_{ox_2}}{2c_2}\left(\sqrt{1 + \frac{Ec_2}{Rqn_{ox_2}}} - 1\right).$$

At temperatures $T_2 > T_{2\gamma}$ the Q_c and Q_1 curves do not touch, i.e., degeneration occurs — the case considered thoroughly in [1].

Consideration of the effect of temperature on ρ, D, and λ yields more realistic results, agreeing with experiment as to particle temperatures [4]. In this case the Semenov conditions take on the form

$$\rho_{2*}\frac{T_*}{T_1}qn_{ox2}\left[\frac{\exp(E/RT_1)}{k_0}+\frac{dc_2\rho_{2*}T_*^{n+1}}{\mathrm{Nu}\,\lambda_{2*}T_1^{n+1}}\right]^{-1}=\mathrm{Nu}\frac{\lambda_{2*}}{d}\left(\frac{T_1}{T_*}\right)^n(T_1-T_2), \tag{17}$$

$$\left[\frac{\exp(E/RT_1)}{k_0}+\frac{dc_2\rho_{2*}T_*^{n+1}}{\mathrm{Nu}\,\lambda_{2*}T_1^{n+1}}\right]^{-2}\left[\frac{E\exp(E/RT_1)}{RT_1k_0}+\right.$$

$$\left.+\frac{(n+1)dc_2\rho_{2*}T_*^{n+1}}{\mathrm{Nu}\,\lambda_{2*}T_1^{n+1}}\right]=\frac{\mathrm{Nu}\,\lambda_{2*}T_1^{n+1}}{dn_{ox2}qT_*^{n+1}}[T_1+n(T_1-T_2)]+\left[\frac{\exp(E/RT_1)}{k_0}+\frac{dc_2\rho_{2*}T_*^{n+1}}{\mathrm{Nu}\,\lambda_{2*}T_1^{n+1}}\right]^{-1}. \tag{18}$$

From Eq. (17) we find

$$d=\mathrm{Nu}\frac{\lambda_{2*}T_1^{n+1}c_2(T_1-T_2)}{c_2\rho_{2*}k_0T_*^{n+1}[qn_{ox2}-c_2(T_1-T_2)]}\exp\frac{E}{RT_1} \tag{19}$$

which when substituted in Eq. (6) yields the equation

$$\frac{[qn_{ox2}-c_2(T_1-T_2)]}{qn_{ox2}}\left\{(T_1-T_2)^2-(T_1-T_2)\frac{n_{ox2}q}{c_2}+\frac{n_{ox2}qRT_1^2}{c_2E[1-RT_1(n+1)/E]}\right\}=0, \tag{20}$$

which allows determination of T_{1i} and T_{1e} and then, with use of Eq. (19), d_i and d_e.

In Fig. 2 the functions obtained by calculation with Eqs. (19) and (20) indicate the necessity of considering the effect of temperature on the transport coefficients and gas density.

The calculation was performed for the same conditions and anthracite properties as the Q_c and Q_l calculations.

Approximate analysis with the assumption that $4c_2RT_1^2/qn_{ox_2}E[1-RT_1(n+1)/E] < 1$ leads to Eqs. (13) and (15) for T_{1i} and T_{1e}, which produce large errors when used to determine critical particle diameters.

NOTATION

T, temperature; d, particle diameter; λ, thermal conductivity; c, specific heat; ρ, density; D, diffusion coefficient; n_{ox}, oxidizer concentration; q, thermal effect of reaction per unit mass of oxidizer; E, activation energy; k_0, preexponential factor; Q, specific thermal capacity; R, universal gas constant; ξ, relative heat liberation; γ, critical condition degeneration parameter; Nu, Nusselt number. Subscripts: 1, particle; 2, gaseous oxidizer; c, chemical reaction; l, heat loss; m, maximum; i, ignition; e, extinction; *, at fixed temperature of T_* = 273 K.

LITERATURE CITED

1. A. G. Makarenko, B. I. Khaikin, and S. I. Khudyaev, Fiz. Goreniya Vzryva, 18, No. 3, 3-9 (1983).
2. V. V. Pomerantsev (ed.), Fundamentals of Practical Combustion Theory [in Russian], Leningrad (1986).
3. A. N. Zolotko, Theory of Inflammation (Handbook) [in Russian], Odessa (1985).
4. V. I. Babii and I. P. Ivanova, Teploenergetika, No. 12, 34-37 (1969).