ON THE THEORY OF COMBUSTION STABILITY OF POWDERS

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The problem of the combustion stability of powders and explosives was first examined by Ya. B. Zel'dovich [1] on the basis of his theory of the mechanism of combustion of these substances. It was established that steady-state combustion of a powder is possible only for $k < 1$, where $k = \beta (T_S - T_0)$, $\beta = (\partial \ln U/\partial T_0)_p$ is the temperature coefficient of the burning rate U, T_0 is the initial temperature, and T_S is the temperature at the gasification surface. Physically, this implies that steady-state combustion of a powder is possible if the temperature gradient at the surface of the condensed phase (k-phase) does not exceed a certain value; a powder which is not hot enough cannot burn.

Subsequent experimental investigations have shown, however, that this combustion stability criterion is not always satisfied [2-4]. The discrepancy between theory and experiment can be associated, in particular, with neglect of the exothermic reaction in the k-phase.

Here the combustion stability of a powder is investigated by the method of small perturbations, taking into account the heat release in the k-phase and assuming that the combustion zone in the gas and the region of chemical reaction in the k-phase directly adjacent to the gasification surface are inertialess. The stability condition is obtained for the two possible combustion regimes with reaction in the k-phase discussed in [6, 7] (T_S- and Q-regimes), and for two different types of reaction. In the case of the Q-regime it is assumed that gasification of the k-phase takes place as a result of an exothermic reaction when the intrinsic heat release, which characterizes the burning depth, becomes equal to a specified value Q_1. In this case in the nonstationary regime the temperature at the gasification surface does not remain constant. In the T_S-regime it is assumed that gasification of the k-phase proceeds at a certain definite temperature (depending, possibly, on the pressure), which is attained thanks to heat supplied from the gas phase and as a result of intrinsic heat release, the quantity of heat released in the k-phase in the nonstationary regime being a variable.

Note that the question of the effect of heat release in the k-phase and the change of surface temperature on the stability of combustion of a powder in the Q-regime with a zero-order exothermic reaction in the k-phase, where the region of combustion in the gas and the zone of chemical reaction in the k-phase are assumed inertialess, has recently been investigated in [5]. The results contained in §2 of the present paper correspond to the case considered in [5]. The conclusions are not the same. Obviously, this discrepancy is associated with the fact that the authors of [5], who used the method of Zel'dovich and Frank-Kamenetskii to derive a formula for the rate of gasification of the k-phase (this leads to a relation between the rate of gasification, heat flux from the gas phase, and the surface temperature) assumed that under nonstationary conditions perturbation of the rate of gasification does not depend on perturbation of the heat flux from the gas phase.

§ 1. Formulation of the Problem

Stability in a two-stage combustion model is considered. The combustion zone is shown schematically in the figure. The temperature gradients at the boundaries of the reaction zone in the k-phase are denoted by φ_{S0} and φ_{S1}. It is assumed that the temperature dependences of the chemical reaction rates $\Phi_1(T)$ and $\Phi_2(T)$ (in the k-phase and in the gas) are such that the reactions proceed mainly within narrow temperature ranges close to T_S and T_2 in the regions $x_1 < x < 0$ and $x_2 < x < x_3$, respectively (T_2 is the temperature of the combustion products). A quantity of heat Q_1 is released in the k-phase, and a quantity Q_2 in the gas phase. The total heat release is determined by the initial chemical energy of the fuel and is equal to $Q_1 + Q_2 = \text{const}$. The region $0 < x < x_2$ is the zone of preheating in the gas. It is assumed that the characteristic time of processes in the zone $x_1 < x < x_3$ is small compared with the time of reconstruction of the thermal layer in the preheating zone in the k-phase, occupying the region $-\infty < x < x_1$. It follows from this assumption and from the equality $\varkappa = D$, where D and $\varkappa$ are the diffusion coefficient and thermal diffusivity of the gas, that at any instant the concentration and temperature fields in the gas are similar. In relation to linearization it is assumed that the time-dependence of all the perturbations is described by the multiplier $\exp(\omega t)$.

§ 2. Combustion Stability in the Q-model with a Zero-order Reaction in the k-phase

In accordance with the assumption concerning an inertialess reaction zone in the k-phase, we shall use the Zel'dovich-Frank-Kamenetskii approximation [8] in order to determine the rate of gasification under nonstationary conditions.

In the case in question, this approximation leads to the following equations for the mass rate of gasification:

$$\lambda_1\varphi_{S0} = \sqrt{\lambda_1^2\varphi_{S1}^2 + A_1(T_S)} \qquad \left(A_1(T_S) = 2\lambda_1 h_1 \int\limits_{T_0}^{T_S} \Phi_1(T)\, dT\right), \tag{2.1}$$

$$\lambda_1\varphi_{S0} - \lambda_1\varphi_{S1} = mQ_1 , \tag{2.2}$$

where λ_1 is the thermal conductivity, h_1 is the heat of reaction in the k-phase. After eliminating the quantity φ_{S1} from (2.1) and (2.2), we obtain

$$mQ_1(2\lambda_1\varphi_{S0} - mQ_1) = A_1(T_S). \tag{2.3}$$

Linearizing (2.3) for the condition Q_1 = const, we find

$$(1-\mu)\frac{\delta m}{m} - z_1\frac{\delta T_S}{T_S - T_0} + \frac{\delta\varphi_{S0}}{\varphi_{S0}} = 0 , \tag{2.4}$$

$$\left(\mu = \frac{Q_1}{c_1(T_S - T_0)} , \; z_1 = \frac{\lambda_1 h_1 \Phi_1(T_S)}{m^2 c_1 Q_1}\right).$$

For the mass burning rate in the gas we have

$$mQ_2 = \sqrt{A_2}, \qquad A_2(T_2) = 2h_2 \int\limits_{T_S}^{T_2} \lambda_2\Phi_2(T)\, dT . \tag{2.5}$$

Note that here $Q_2 > h_2$, since $Q_1 < h_1$, while the mechanism of release of heat $h_1 - Q_1$ after gasification is not considered*.

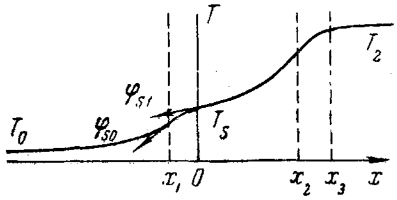

Fig. 1.

Linearizing Eq. (2.5) for the condition Q_2 = const, taking into account $\Phi_2(T_2) \gg \Phi_2(T_S)$, we obtain

$$\frac{\delta m}{m} - z_2\frac{\delta T_2}{T_2} = 0 \qquad \left(z_2 = \frac{h_2\lambda_2\Phi_2(T_2)\,T_2}{m^2 Q_2^2}\right). \tag{2.6}$$

In the quasistationary approximation, the law of conservation of energy in the region $x_1 < x < x_3$ may be written, following [1], in the form

$$m(c_1 T_S + Q_1 + Q_2) - \lambda_1\varphi_{S0} = mc_2 T_2 , \tag{2.7}$$

where c_1 and c_2 are the specific heats of the k-phase and the gas at constant pressure.

On linearizing (2.7) and taking into account the condition $Q_1 + Q_2$ = const, we obtain:

$$\frac{\delta m}{m} + \frac{\delta T_S}{T_S - T_0} - \frac{1}{\tau}\frac{\delta T_2}{T_2} - \frac{\delta\varphi_{S0}}{\varphi_{S0}} = 0 , \qquad \left(\tau = \frac{c_1(T_S - T_0)}{c_2 T_2}\right). \tag{2.8}$$

We shall obtain one more relation between the perturbations of the mass velocity δm, the temperature gradient $\delta\varphi_{S0}$, and the surface temperature δT_S from the solution of the problem of the reconstruction of the thermal layer in the region of the k-phase, where the chemical reaction rate is negligibly small, for small changes in the surface velocity assuming that the temperature at the point x_1 is equal to the surface temperature T_S . For perturbations depending on time as $\exp(\omega t)$, this solution has the form:

$$\delta T(x) = -\frac{T_S - T_0}{\Omega}\frac{\delta m}{m}\exp\left(\frac{Ux}{\varkappa_1}\right) + B_1\exp\left(\frac{U\beta_1 x}{2\varkappa_1}\right) + B_2\exp\left(\frac{U\beta_2 x}{2\varkappa_1}\right) \tag{2.9}$$

$$(\Omega = \varkappa_1\omega / U^2, \; \beta_{1,2} = 1 \pm \sqrt{1 + 4\Omega}),$$

where B_1 and B_2 are arbitrary constants, $\varkappa_1$ is the thermal diffusivity of the k-phase, and U is the rate of linear displacement on the surface. From the condition $\delta T(-\infty) = 0$ it follows that $B_2 = 0$. We find B_1 from the boundary conditions for $x = 0$ and establish the required relation:

$$\frac{\beta_2}{2\Omega}\frac{\delta m}{m} - \frac{\beta_1}{2}\frac{\delta T_S}{T_S - T_0} + \frac{\delta\varphi_{S0}}{\varphi_{S0}} = 0. \tag{2.10}$$

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*In proofreading, B. V. Novozhilov pointed out that if in (2.5) it is assumed that $Q_2 = h_2$ [which is physically more justifiable than (2.5)], then the stability conditions for the T_S-model obtained in §3 and 5 assume the form $\varepsilon < 1$, i.e., they coincide with the stability criterion for Zel'dovich's model.

From Eqs. (2.4), (2.6), (2.8) and (2.10) we obtain the characteristic equation for Ω :

$$\gamma\Omega + 2(\varepsilon - 1)\Omega + \varepsilon = (\gamma\Omega + \varepsilon)\sqrt{1 + 4\Omega}$$
$$\left(\gamma = \frac{1 - (2 - \mu)\varepsilon}{1 - z_1}, \quad \varepsilon = \tau z_2\right).$$

From an analysis of the roots of Eq. (2.1) it follows that the stability condition for the combustion regime investigated has the form:

$$(\varepsilon - 1)^2 - \gamma(\varepsilon + 1) < 0. \tag{2.12}$$

This inequality is fulfilled only for $\gamma > 0$. The quantity z_1 entering into γ can be represented in the form:

$$z_1 = \frac{1}{2}(2 - \mu) M_1, \qquad M_1 = \Phi_1(T_S)(T_S - T_0)\left[\int_{T_0}^{T_S} \Phi_1(T)\, dT\right]^{-1}. \tag{2.13}$$

With the ordinary assumptions of combustion theory concerning the properties of the function $\Phi_1(T)$ (positiveness, monotonic increase, continuity), the quantity M_1 characterizes the "sharpness" of the temperature dependence of the chemical reaction rate. Obviously, $M_1 > 1$.

For $\Phi_1 = D \exp(-E_1/RT)$, an approximate estimate using the inequality $E_1/RT \gg 1$ gives:

$$M_1 \approx E_1(T_S - T_0)/RT_S^2.$$

The chemical reaction zone in the k-phase is assumed to be inertialess, and therefore the results will be valid only for sufficiently large activation energies E_1. For $z_1 > 1$, stability condition (2.12) is fulfilled only for $\varepsilon > 1/(2 - \mu)$. This condition is necessary but not sufficient. If $z_1 > 3 - \mu$, it can be shown that for combustion stability the inequality $\varepsilon < \varepsilon_2$, $(\varepsilon_1 < \varepsilon_2)$, where $\varepsilon_{1,2}$, the roots of the quadratic trinomial (2.12), must also be satisfied.

In comparing the stability condition for the model considered with the stability condition for Zel'dovich's combustion model, it should be borne in mind that for a heat release in the k-phase tending to zero, the Q-model does not go over into the Zel'dovich model, and condition (2.12) into the corresponding condition for the parameter k.

§ 3. Combustion Stability in the T_S-model with a Zero-Order Reaction in the k-Phase

In this case, as distinct from the Q- model considered above, the equations are linearized for the condition T_S = =const. From Eq. (2.3) we obtain:

$$q(1 - \mu)\frac{\delta m}{m} + (1 - \mu)\frac{\delta Q_1}{Q_2} + q\frac{\delta\varphi_{S0}}{\varphi_{S0}} = 0 \qquad \left(q = \frac{Q_1}{Q_2}\right). \tag{3.1}$$

Similarly, from Eq. (2.5)

$$\frac{\delta m}{m} - \frac{\delta Q_1}{Q_2} - z_2\frac{\delta T_2}{T_2} = 0. \tag{3.2}$$

Equations (3.1) and (3.2), together with Eqs. (2.8) and (2.9), in which it is necessary to assume $\delta T_S = 0$, form a closed system whose characteristic equation has the form:

$$\frac{\sqrt{1 - 4\Omega} - 1}{2\Omega} = \frac{(1 - \mu)(\varepsilon - 1 - q)}{(1 - \mu)\varepsilon + q}. \tag{3.3}$$

Investigation of the roots of Eq. (3.3) shows that the T_S combustion regime with a zero-order reaction in the k-phase is stable for

$$\frac{\varepsilon(1 - \mu) + q}{(1 + q)(1 - \mu) + q} < 1, \quad \text{or} \quad \varepsilon < 1 + q. \tag{3.4}$$

Note that in the case $q = 0$, corresponding to the absence of heat release in the k-phase, criterion (3.4) coincides with the stability condition obtained by Zel'dovich. It can be seen from (3.4) that in the given case an increase in heat release in the k-phase extends the range of values of ε corresponding to stable combustion.

§ 4. Combustion Stability in the Q-model with a First-Order Reaction in the k-Phase

For steady-state propagation of the front of a first-order exothermic reaction in the k-phase we have the relations:

$$mQ_1 = h_1 \int_{-\infty}^{0} a(x)\,\Phi_1[T(x)]\,dx\,,$$

$$h_1 a(x) = h_1 a_0 - c_1(T - T_0) + \frac{\lambda_1}{m}\frac{dT}{dx}\,, \tag{4.1}$$

where $a(x)$ is the concentration of the substance reacting in the k-phase, $a(-\infty) = a_0$. Assuming that the chemical reaction zone in the k-phase is narrow and averaging the temperature gradient over this zone, an approximate formula can be obtained for the propagation velocity of the reaction front:

$$mQ_1(2\lambda_1\varphi_{S0} - mQ_1) = 2\lambda_1 \int_{T_0}^{T_S} [h_1a_0 - c_1(T - T_0)]\,\Phi_1(T)\,dT + \frac{\lambda_1(2\lambda_1\varphi_{S0} - mQ_1)}{m} \int_{T_0}^{T_S} \Phi_1(T)\,dT, \tag{4.2}$$

Linearizing Eq. (4.2) for the condition Q_1 = const, we obtain:

$$\left(1 - \mu + \frac{A}{\mu}\right)\frac{\delta m}{m} - z_{11}\frac{\delta T_S}{T_S - T_0} + \left(1 - \frac{A}{\mu}\right)\frac{\delta\varphi_{S0}}{\varphi_{S0}} = 0$$

$$\left(z_{11} = \frac{\lambda_1\Phi_1(T_S)(2h_1a_0 - Q_1)}{2m^2c_1Q_1}\,,\quad A = \frac{1}{m\varphi_{S0}}\int_{T_0}^{T_S}\Phi_1(T)\,dT\right). \tag{4.3}$$

It is easy to obtain the characteristic equation for Ω from Eqs. (4.3), (2.6), (2.8) and (2.10) in a form identical with Eq. (2.11), but with the parameter γ in the form:

$$\gamma_1 = \left[1 - (2 - \mu)\,\varepsilon - \frac{A}{\mu}\right] \Big/ \left[1 - z_{11} - \frac{A}{\mu}\right].$$

Correspondingly, in the case in question the condition for combustion stability will also have the form of inequality (2.12) with $\gamma = \gamma_1$.

§ 5. Combustion Stability in the T_S-model with a First-Order Reaction in the k-Phase

Linearizing Eqs. (2.4) for T_S = const gives

$$\left(1 - \mu + \frac{A}{\mu}\right) q\,\frac{\delta m}{m} + \left(1 - \mu + \frac{A}{2}\right)\frac{\delta Q_1}{Q_2} + \left(1 - \frac{A}{\mu}\right) q\,\frac{\delta\varphi_{S0}}{\varphi_{S0}} = 0. \tag{5.1}$$

The closed system of equations is now formed by equations (5.1), (3.2) and (2.8), (2.10), in which it is necessary to substitute $\delta T_S = 0$. Equating the determinant of this system to zero, we obtain the characteristic equation for Ω, which has the form:

$$\frac{\sqrt{1 + 4\Omega} - 1}{2\Omega} = 1 - \frac{1}{\gamma_2}\,,\quad \gamma_2 = \frac{(1 - \mu + {}^1\!/_2 A)\,\varepsilon + (1 - \mu^{-1}A)\,q}{(2 - \mu)\,q + (1 - \mu + {}^1\!/_2 A)}\,. \tag{5.2}$$

From an analysis of the roots of Eq. (5.2) it follows that the steady-state T_S combustion regime with a first-order reaction in the k-phase is stable provided that

$$\varepsilon < 1 + \frac{1 - \mu + \mu^{-1}A}{1 - \mu + {}^1\!/_2 A}\,q\,. \tag{5.3}$$

Comparing conditions (3.4) and (5.3), we note that taking into account burnup of the reactant in the k-phase reaction extends the limits of combustion stability of the powder.

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