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Abstract

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ON THE THEORY OF COMBUSTION OF CONDENSED SYSTEMS

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Experimental data indicate that gasification of the condensed phase of powders and certain explosives during combustion is accompanied by appreciable heat release ([1–3]). In the theory of powder combustion developed earlier by Ya. B. Zel' dovich ([4]), this effect was not taken into account, while later works ([5–7]) were based on the assumption that the exothermic reaction occurring in the condensed phase is of zero order, i.e., does not depend on the concentration of the reacting substance. Experimentally ([1–3]) it has been found that the depth of transformation of the condensed phase before its gasification may be rather large ($\sim 30\%$); therefore it is of interest to take this fact into account at least qualitatively.

We investigate the question of the existence and uniqueness of the solution of the problem of combustion of the condensed phase, assuming that the reaction in the condensed phase is monomolecular, and considering that the influence of the gas phase is manifested in the presence of a heat flux from the gas phase into the condensed phase.

The equations describing the processes in the condensed phase and the boundary conditions have the form

$$\lambda \frac{d^2T}{dx^2} - mc\frac{dT}{dx} + ha\Phi(T) = 0; \tag{1}$$

$$m\frac{da}{dx} + a\Phi(T) = 0, \qquad -\infty \leqslant x \leqslant 0; \tag{2}$$

$$x = -\infty, \qquad T = T_0, \qquad a = a_0; \tag{3}$$

$$x = 0, \qquad T = T_s, \qquad \lambda\frac{dT}{dx} = q_s; \tag{4}$$

where T is temperature, a is concentration, m is the mass burning rate, c is heat capacity, λ is the coefficient of thermal conductivity, h is the heat effect of the reaction, q_s is the heat flux at the "hot"boundary, and $\Phi(T)$ is the dependence of the chemical reaction rate on temperature. With respect to the function $\Phi(T)$, we assume that $\Phi(T) = 0$ for $T_0 \leqslant T \leqslant T_\varepsilon$, and that $\Phi(T)$ is a monotonically nondecreasing function for $T > T_\varepsilon$, where T_ε is the "cutoff" parameter (see ([8])).

We note that the formulation of the boundary condition at the hot boundary in the form (4) is not the only possible one ([9]).

Substituting the expression for $a\Phi(T)$ from (2) into (1) and integrating over the interval $(-\infty, x)$, we obtain

$$a(x) = a_0 - \frac{c}{h}(T - T_0) + \frac{\lambda}{mh}\frac{dT}{dx}. \tag{5}$$

Using (5), we reduce the system of equations (1), (2) to a single equation

$$\frac{d^2T}{dx^2} - \left[\frac{mc}{\lambda} - \frac{\Phi(T)}{m}\right]\frac{dT}{dx} + \frac{\Phi(T)}{\lambda}\left[ha_0 - c(T - T_0)\right] = 0. \tag{6}$$

Denoting

$$p = \lambda\frac{dT}{dx}; \qquad \varphi(T) = c\lambda\Phi(T); \qquad T_* = T_0 + \frac{ha_0}{c}; \qquad \omega = mc,$$

we reduce problem (1)–(4) to the form:

$$\frac{dp}{dT} = \omega - \frac{\varphi(T)}{\omega} - \frac{\varphi(T)(T_* - T)}{p}; \tag{7}$$

$$p = 0 \quad \text{for } T = T_0; \tag{8a}$$

$$p = q_S \quad \text{for } T = T_S. \tag{8b}$$

To prove the existence and uniqueness of the solution of the boundary-value problem (7), (8), we distinguish the cases: 1) $T_* > T_S$; 2) $T_\varepsilon < T_* \leqslant T_S$; 3) $T_* \leqslant T_\varepsilon$.

Case 1). Consider, along with equation (7), the auxiliary equation

$$\frac{dp_1}{dT} = \omega - \frac{\varphi(T)(T_* - T)}{p}. \tag{9}$$

The problem of finding a solution of equation (9) with conditions (8) formally coincides with the problem of combustion of the condensed phase in the case of a zero-order reaction, which always has a unique solution[9]. Denote the solution of equation (9) with conditions (8) by $p_1(T), \omega_1$.

The point $T = T_S,\ p = q_S$ is a regular point of equations (7), (9), and for $\omega = \omega_1$ one integral curve of these equations passes through it; moreover, from the form of the equations it follows that

$$\frac{dp_1}{dT} > \frac{dp}{dT}.$$

Thus, the curve $p(T)$ for $\omega = \omega_1$ lies above the curve $p_1 T$.

It follows from equation (7) that the curve $p(T)$ cannot have a vertical tangent for $T_\varepsilon < T < T_S,\ p > 0$, and has no vertical asymptote. Therefore, the integral curve of equation (7) for $\omega = \omega_1$, passing through the point $T = T_S,\ p = q_S$, intersects the line $T = T_\varepsilon$ at a point $p(T_\varepsilon) \neq \infty$. The further course of the proof is essentially no different from the method of Ya. B. Zel' dovich[8], also used in[9,10]. Considering the function $p_\omega(T) = \partial p/\partial\omega$ on the interval (T_ε, T_S), we find that problem (7)–(8) always has a unique solution for some finite $\omega > \omega_1$.

In the case under consideration, a regime with $q_S = 0$ (so-called flameless combustion) is possible. Then

$$\left.\frac{dp}{dT}\right|_{T=T_S} = \left.\frac{dp_1}{dT}\right|_{T=T_S} = -\infty,$$

but here also the curve $p_1(T)$ passes below the curve $p(T)$, and although the equation for $p_\omega(T)$ has a singular point at $T = T_S$, the inequality $p_\omega(T) \leqslant 0$ is satisfied, so that the proof remains valid.

Case 2). Within the temperature-variation interval the function $\varphi(T)(T_* - T)$ changes sign at the point $T = T_*$; therefore the point $T = T_*,\ p = 0$ is a singular point of equation (7)—a saddle. The slopes of the separatrices at this point are equal to

$$p'_{(1)}(T_*) = \omega; \qquad p'_{(2)}(T_*) = -\frac{\varphi(T_*)}{\omega}. \tag{10}$$

The equation of the separatrix having positive slope is

$$p_0(T) = \omega(T - T_*). \tag{11}$$

We shall now show that in the present case the solution of problem (7), (8) exists and is unique if q_S is greater than some value q_{cr}; otherwise, i.e., for $q_S < q_{\mathrm{cr}}$, there are no solutions. Denote by ω_* the value of ω for which the solution of equation (7) satisfies conditions (8a) and $p(T_*) = 0$ (see Fig. 1). The existence

Fig. 1

Figure 1: Fig. 1

and uniqueness of such a solution can be established by a method similar to that applied in case 1. We further verify that

$$q_{\mathrm{cr}} = \omega^*(T_S - T_*). \tag{12}$$

Indeed, for $q_S < q_{\mathrm{cr}}$, the integral curves passing above the separatrix $p_0(T)$ and satisfying the condition at the "hot" boundary appear only when $\omega < \omega_*$. However, for such values of ω these integral curves cannot satisfy the condition at the "cold" boundary, because, as follows from the properties of the function $p_\omega(T)$, the left branch of the separatrix, lying in the positive half-plane, does not decrease with decreasing ω at all points of the interval (T_ε, T_*), whereas the solution of equation (7) with condition (8a) on the interval (T_0, T_ε), having the form $p = \omega(T - T_0)$, obviously decreases with decreasing ω.

To verify the existence and uniqueness of the solution of problem (7), (8) for $q_S > q_{\mathrm{cr}}$, consider the solutions of equation (7) on the interval (T_0, T_*) with the conditions $p = 0$ at $T = T_0$ and $p = q_*$ at $T = T_*$. As follows from case 1, such solutions always exist for $q_* > 0$. Taking into account the properties of the function $\varphi(T)$, one may assert that each of these solutions can be continued to the right up to any finite T_S. This continuation necessarily intersects the line $T = T_S$, since it lies between the straight lines $p = \omega(T - T_0)$ and $p = \omega(T - T_*)$.

Fig. 1

Let $q_*^{(1)} < q_*^{(2)}$. Then the solutions of equation (7) with the conditions $p(T_0) = 0$ and $p(T_*) = q_*^{(i)}$, where $i = 1, 2$, correspond to $\omega_1 < \omega_2$. The impossibility of the intersection of these curves for $T < T_*$ follows from the proof of case 1. The supposition that the curves intersect at some point lying to the right of $T = T_*$ leads to a contradiction. Then, from the position of the curves near the point $T = T_\varepsilon$, it follows that the upper curve corresponds to the larger ω, while from the properties of the function p_ω it follows that the upper curve must correspond to the smaller value of ω.

Consequently, integral curves passing through different points on the straight line $T = T_*$ do not intersect and correspond to different ω. In this case, as q_* increases, ω increases and $p(T_S) = q_S$. The growth of q_S occurs no more slowly than $\omega(T_S - T_*)$. Therefore, for some finite ω contained within the limits $\omega_* < \omega < q_S/c(T_S - T_*)$, one will have $p(T_S) = q_S$, and all the conditions of problem (7), (8) will be satisfied. As $T_* \to T_\varepsilon$, $\omega_* \to 0$, and consequently $q_{\mathrm{cr}} \to 0$.

Case 3). To prove existence and uniqueness of the solution in this case, note that for

$$\omega = \frac{q_S}{c(T_S - T_*)}$$

the straight lines $p = \omega(T - T_0)$ and $p = \omega(T - T_*)$ are solutions of equation (7) with condition (8a) on the segment $T_0 \leq T \leq T_\varepsilon$ and with condition (8b) on the segment $T_\varepsilon < T < T_S$, respectively. By decreasing ω below the value indicated above, we see that the solution exists and is unique for all $q_S > 0$.

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Note: Figure translations are in progress. See original paper for figures.