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Abstract

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ANALYSIS OF MATHEMATICAL MODELS OF COMBUSTION OF THE CONDENSED PHASE

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A characteristic feature of the combustion process in condensed systems is the multistage nature of the transformation of the fuel in the combustion front. Therefore the theory of combustion faces the task of studying the individual stages, their interaction with one another, and identifying the leading stage (if there is one). In works ([1]-[3]) the substantial role of an exothermic reaction in the condensed phase was demonstrated experimentally. It has been established that about 70% of the heat required to heat the substance to the temperature of the burning surface is acquired by the c-phase through its self-heating. In particular, the so-called flameless combustion of nitroglycerine powders was investigated, in which propagation of the combustion front is maintained by only one reaction, taking place in the condensed phase.

In work ([4]) it was shown that, as the external pressure increases, the heat released by the chemical reaction in the c-phase increases. Therefore the study of the laws governing combustion of the c-phase does not lose its significance even in the presence of well-developed later stages of combustion. Theoretical investigations of the role of the c-phase in the combustion process were carried out in works ([5]-[9]).

In the present work we consider the question of the existence and uniqueness of the solution of the equations describing the process of combustion of the c-phase, and we give a generalization of the well-known theorem of Ya. B. Zel' dovich ([8]) on the existence and uniqueness of the solution in the thermal theory of flame propagation in gases to the case of combustion of the c-phase.

In one of the possible formulations, the question of combustion of the c-phase reduces to the solution of the following boundary-value problem:

$$\lambda \frac{d^2T}{dx^2} - mc\frac{dT}{dx} + h\Phi(T) = 0, \qquad -\infty \le x \le 0;$$

$$T(-\infty) = T_0; \qquad T(0) = T_s; \qquad \lambda \left.\frac{dT}{dx}\right|_{x=0} = q_s. \tag{1}$$

Here h is the enthalpy of the c-phase; $\Phi(T)$ is the volumetric rate of the chemical reaction, which is assumed not to depend on the concentration of the reacting substance; T is temperature. The meaning of the remaining notation is clear from the formulation. The most essential feature distinguishing system (1) from the corresponding system describing thermal propagation of flame in a gas is that the function $\Phi(T_s)$, generally speaking, does not vanish at the "hot" boundary of the c-phase, i.e. $\Phi(T_s) \neq 0$. In this case the chemical reaction is terminated by an extraneous factor—the gasification of the c-phase. In addition, the problem of combustion of the c-phase is considered on the semi-infinite interval $(-\infty, 0)$; therefore the value of the temperature gradient at the "hot" boundary is not determined by prescribing a finite value of the temperature at this boundary, as was the case for gas combustion.

Introducing the variables $\tau = \dfrac{T - T_0}{T_s - T_0}$, $\xi = x\sqrt{2N}$, $p = d\tau/d\xi$, where

$$N = \frac{h}{\lambda(T_s - T_0)} \int_0^1 \Phi(\tau)\, d\tau,$$

and denoting

$$v = \frac{mc}{\lambda\sqrt{2N}}, \qquad \delta_s = \frac{q_s}{\lambda(T_s - T_0)\sqrt{2N}},$$

$$\varphi(\tau) = \frac{h}{\lambda(T_s - T_0)} \frac{\Phi(\tau)}{2N},$$

from (1) we obtain

$$\frac{dp}{d\tau} = v - \frac{\varphi(\tau)}{p}, \qquad 0 \leq \tau \leq 1;$$

$$p(0) = 0; \qquad p(1) = \delta_s : \qquad \delta_s \geq 0. \tag{2}$$

It is assumed that the function $\varphi(\tau)$ satisfies the conditions

$$\varphi(\tau) = \begin{cases} 0 & \text{for } 0 \leq \tau < \varepsilon, \\ > 0 & \text{for } \varepsilon < \tau \leq 1; \end{cases} \qquad \int_0^1 \varphi(\tau)\, d\tau = \frac{1}{2}, \tag{3}$$

where ε is the "cutoff" parameter (see (8)).

We shall assume that flameless combustion corresponds to the case $\delta_s = 0$. It is characteristic that in the problem of k-phase combustion the point $\tau = 1$, $p = \delta_s$ is not a singular point of equation (2). As $\tau \to 1$,

$$\frac{dp}{d\tau} \to v - \frac{\varphi(1)}{\delta_s},$$

i.e.

$$\left.\frac{dp}{d\tau}\right|_{\tau=1}$$

is a finite, prescribed quantity for all finite values of δ_s. In the case of flameless combustion,

$$\left.\frac{dp}{d\tau}\right|_{\tau=1} = -\infty.$$

From consideration of the field of integral curves of equation (2) and, in particular, of the position of the zero-slope isocline $p = \varphi(\tau)/v$, it is clear that any integral curve passing through the point $p(1) = \delta_s$, for a finite value of v, necessarily intersects the straight line $\tau = \varepsilon$ at some finite point. For $v = 0$, the integral curve $p_0(\tau)$ satisfying the condition $p(1) = \delta_s$ has the form

$$p_0(\tau) = \left[\delta_s^2 + 2\int_\tau^1 \varphi(x)\,dx\right]^{1/2}, \qquad p_0(\varepsilon{+}0) = \left[\delta_s^2 + 1\right]^{1/2} > 0, \qquad \varepsilon \le \tau \le 1. \tag{4}$$

On the interval $(0, \varepsilon)$, the solution of equation (2) with the condition $p_0(0) = 0$ is $p_0(\tau) = 0$, and, consequently, $p_0(\varepsilon - 0) = 0$. Following further the work (8), let us consider the quantity $p_v = \partial p/\partial v$. From (2) we have

$$\frac{dp_v}{d\tau} = 1 + \frac{\varphi(\tau)}{p^2(\tau)}\,p_v. \tag{5}$$

Since solutions satisfying the condition $p(1) = \delta_s$, independently of v, are being considered, $p_v(1) = 0$. Consequently, if $\delta_s \neq 0$, then

$$\left.\frac{dp_v}{d\tau}\right|_{\tau=1} = 1.$$

The values of the function $p_v(\tau)$, when moving from the point $\tau = 1$, $p_v = 0$ from right to left, fall into the lower half-plane and cannot enter the upper half-plane for $\varepsilon \le \tau \le 1$. Consequently, $p_v(\tau) \le 0$ and $p_v(\varepsilon + 0) \le 0$. Thus, one may assert that the quantity $p(\varepsilon + 0)$ does not exceed its value $p_0(\varepsilon + 0) = [1 + \delta_s^2]^{1/2}$ as v increases from zero. At the same time, since for $0 \le \tau \le \varepsilon$, $p(\tau) = v\tau$, the quantity $p(\varepsilon - 0) = v\varepsilon$, i.e. it increases with increasing v at a finite rate. Hence it follows that, for some finite value $v = v_*$, $p(\varepsilon + 0) = p(\varepsilon - 0)$, i.e. there exists a unique (by virtue of the monotonic character of the variation of $p(\varepsilon + 0)$ and $p(\varepsilon - 0)$ with changing v) solution of system (2).

The case of flameless combustion, when $\delta_s = 0$, is special. With

then the point $(1, 0)$ will be a singular point of equation (5). However, in this case as well it is possible to determine the slope of the curve $p_\nu(\tau)$ at $\tau = 1$. For this it is enough to note that, as $\tau \to 1$, by virtue of the equation $p\,dp/d\tau - \nu p + \varphi = 0$, the quantity $p\,dp/d\tau \to -\varphi(1)$, i.e., is continuous and remains finite. Therefore, resolving the indeterminacy in the right-hand side of equation (5), we obtain:

$$\lim_{\tau\to1} \frac{\varphi(\tau)p_\nu(\tau)}{p^2(\tau)} = \varphi(1) \lim_{\tau\to1} \frac{dp_\nu/d\tau}{2p\,dp/d\tau} = -\frac{1}{2}\left.\frac{dp_\nu}{d\tau}\right|_{\tau=1};$$

$$\left.\frac{dp_\nu}{d\tau}\right|_{\tau=1} = \frac{2}{3} \quad \text{for } \delta_s = p(1) = 0. \tag{6}$$

Taking (6) into account, the arguments presented above remain valid also in this case. Thus, the existence and uniqueness of system (1) have been established. However, the formulation of the problem of combustion of the k-phase in the form (1) is not the only possible one. The existing experimental data are still insufficient for an unambiguous specification of the conditions under which the k-phase changes its state of aggregation—gasifies. Two, in a certain sense limiting, approaches to this question may be formulated.

Case I is the one for which the theorem of existence and uniqueness was established above. We shall provisionally call it the T_s-model. In this model T_s is a prescribed quantity, analogous to the boiling temperature in the Zel' dovich-Belyaev combustion model (^{5}). The amount of heat Q_k released in the k-phase due to the chemical reaction is not equal to the enthalpy h and is determined from the formulas

$$Q_k = \frac{h}{m}\int_{-\infty}^{0} \Phi(T)\,dx; \qquad q_s - mc(T_s - T_0) + mQ_k = 0. \tag{7}$$

Case II will be called the Q-model. The k-phase gasifies if, as a result of the chemical reaction proceeding in it, a prescribed amount of heat Q_k has been released.

In this model the value of the temperature of the burning surface is determined from the solution of the problem by the formula

$$T(0) = T_0 + \frac{Q_k}{c} + \frac{q_s}{mc}. \tag{8}$$

Fig. 1 and Fig. 2

Figure 1: Fig. 1 and Fig. 2

The boundary-value problem is written in the form

$$p\frac{dp}{d\tau} - \omega p + F(\tau) = 0, \qquad p(0) = 0, \qquad p(\tau_s) = \mu_s, \qquad \tau_s = 1 + \frac{\mu_s}{\omega}, \tag{9}$$

where

$$\tau = \frac{T - T_0}{T_{s1} - T_0}, \qquad T_{s1} = T_0 + \frac{Q_k}{c}, \qquad \omega = \frac{mc}{\lambda}, \qquad p = \frac{d\tau}{dx}, \qquad \mu_s = \frac{cq_s}{\lambda Q_k},$$

$$F(\tau) = \frac{hc}{\lambda Q_k}\,\Phi(\tau).$$

Let us establish the theorem of existence and uniqueness for (9). First consider the case $q_s = 0$. Then $\tau_s = 1$, $p(1) = 0$, and the theorem established for (1) applies. Let this correspond to $\omega = \omega_0$. We shall next verify that, for $q_s \neq 0$, the situation shown in Fig. 1 holds, where curve 1 is the integral curve of equation (9) for $q_s = 0$ and $\omega = \omega_0$, and curve 2 is the integral curve of the same equation for $q_s \neq 0$ and $\omega = \omega_0$. Curve 2 cannot intersect curve 1, since at the point of intersection there would be a singular point of equation (9), whereas no such point exists. Consequently, for $\omega = \omega_0$ curve 2 lies above curve 1 and intersects the line $\tau = \varepsilon$ at some finite point A. Further, by investigating the behavior of the quantities $p(\varepsilon + 0)$ and $p(\varepsilon - 0)$ as ω increases from ω_0, it is not difficult, as before, to con-

to be convinced of the validity of the existence and uniqueness theorem for the Q-model.

Consider the case when the Q- and T_s-models are not mutually exclusive. Let T_0, T_s, and q_s be specified; then there exists a unique value $m = m_1$ and $Q_k = Q_k^1$. If we now assume that the chemical reaction in the k-phase ceases when the heat released as a result of this reaction is equal to $Q_k^2 < Q_k^1$, then the situation shown in Fig. 2 is possible. Since now m is a known quantity,

$$m = \frac{q_s}{c(T_s - T_0) - Q_k^2},$$

Fig. 1 Fig. 2

then from the point O the integral curve reaches the point A with known coordinates $(T_\varepsilon, \omega T_\varepsilon)$. If the integral curve passing through the point A intersects the line BC, parallel to OA, then a “subsurface” regime occurs, in which the reaction ceases at $T_* < T_s$. Since $T_B = T_0 + Q_k/c$, by increasing q_s with unchanged T_s, we can always obtain such a regime. If, in passing from conditions of flameless combustion to conditions of elevated external pressure, T_s remained unchanged, then the “subsurface” regime would be excluded by the very fact of flameless combustion. Since T_s increases with increasing pressure, such a regime is in principle not excluded.

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