

THEORY OF COMBUSTION OF GASES AND CONDENSED SUBSTANCES

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In the investigation of combustion in various systems, additional assumptions often have to be made about the properties of particular quantities owing to the impossibility of obtaining exact solutions of the corresponding equations. For instance, in the investigation of the combustion of powder the temperature gradient on the surface of the condensed phase plays an important role. In the steady state this gradient φ is given by the relationship

$$\varphi = u\lambda^{-1}(T_1 - T_0). \tag{0.1}$$

Here u is the burning rate, λ is the thermal diffusivity, T_1 is the temperature of the surface of the powder, and T_0 is the temperature of the cold powder.

It is important to find out how φ behaves when T_0 changes. When T_0 decreases the factor u decreases, while $(T_1 - T_0)$ increases, and it is very difficult to draw any conclusions regarding the behavior of φ . Zel'dovich in [1, 2] suggested that the gradient φ as a function of T_0 has a maximum and that for each value of φ there are two combustion regimes—one stable (for large T_0) and one unstable (for small T_0). Since at the maximum point $d\varphi/dT_0 = 0$, combustion is regarded as stable if $d\varphi/dT_0 < 0$ and as unstable if $d\varphi/dT_0 > 0$. It has been reported on several occasions [2-5], however, that this criterion is not always satisfied, and various hypotheses as to the possible reasons for this discrepancy have been put forward. In addition, it is of definite interest to analyze the basic assumption of the existence of a maximum of φ . If such an analysis is to be made, the right side of (0.1) will have to be expressed in terms of one variable, u or T_0 , for which, in turn, a relationship between u and T_0 will have to be obtained.

This paper consists of four sections. In §1 the normal propagation of a flame is investigated and a formula relating u to T_0 is derived. In §2 the relationship between u and T_0 in the case of combustion of condensed substances is obtained by a similar method. In §3 the obtained formulas are used to investigate the behavior of the temperature gradient. In §4 the stability of combustion processes is analyzed.

§1. Normal propagation of flame in gases. We know [6, 7] that the normal propagation of flame in a gas when the thermal diffusivity and diffusion coefficient are equal is represented by the differential equation

$$\lambda d^2T/dx^2 + udT/dx + F(T) = 0, \tag{1.1}$$

with boundary conditions

$$T|_{x \rightarrow -\infty} = T_2, \quad T|_{x \rightarrow +\infty} = T_0. \tag{1.2}$$

Here $T(x)$ is the temperature along the x -axis, T_0 is the temperature of cold gas, T_2 is the temperature of the burned gas, and λ is the thermal diffusivity. The flame is propagated in the positive direction of the x -axis. Function $F(T)$ satisfies the conditions: $F(T) = 0$ when $T_0 \leq T \leq T_1$; $F(T) > 0$ when $T_1 < T < T_2$, and $F(T) = 0$ when $T > T_2$. In the interval (T_1, T_2) function $F(T)$ has one maximum. The parameter u characterizes the normal velocity of flame propagation. We have to find the value of this parameter for which there is a solution of problem (1.1) and (1.2).

In [6, 7] the existence of a single value of this parameter was demonstrated. Various methods [6, 8-10] have been proposed for the calculation of u . A formula for the approximate calculation of u is given in [6, 10]:

$$u = \frac{\sqrt{2\lambda J}}{T_1 - T_0}, \quad J = \int_{T_1}^{T_2} F(T) dT. \tag{1.3}$$

This formula is based on neglect of the middle term of Eq. (1.1) in the combustion zone. It is easy to see that formula (1.3) will give a value of u in excess of the exact value. In fact, if the middle term is not

neglected then the integrand in (1.3) will be $F(T) + udT/dx$, which is less than $F(T)$, since $dT/dx < 0$. This becomes particularly appreciable as $T_0 \rightarrow T_1$, since then the value of u from formula (1.3) can become as large as you please; it follows from [11] that u actually has a limit as $T_0 \rightarrow T_1$.

A review of various methods of solving the problem is given in [8]. In [9] numerical integration of the nonstationary system of heat-conduction and diffusion equations was used to find u . In this section we propose a method by which an approximate value of u and the temperature distribution in the flame can be found fairly easily. As the example given at the end of the section shows, the value of u calculated by this method is reasonably close to the exact value. The convenience of this method lies in the fact that the relationship between u and the parameters of the process is obtained in analytical form. We assume that $T|_{x=0} = T_1$; then for $x \geq 0$

$$T|_{x \geq 0} = (T_1 - T_0) \exp(-ux/\lambda) + T_0. \tag{1.4}$$

To find the temperature distribution when $x < 0$ we replace function $F(T)$ by a piecewise-linear function in the interval $[T_1, T_2]$. We perform the linearization in the following way. We take a point T_3 in $[T_1, T_2]$ and construct a triangle with base $[T_1, T_2]$ and its third vertex P situated above the point T_3 . We require the area of the triangle to be equal to the area under the curve $F(T)$, i. e.,

$$S = \int_{T_1}^{T_2} F(T) dT = J.$$

It is obvious that the third vertex is uniquely determined (for a particular choice of T_3). The point T_3 can be chosen at the maximum point of $F(T)$. We denote the function obtained in this way by $F^*(T)$ and we have

$$F^*(T) = \begin{cases} \beta_1(T - T_1) & \text{for } T_1 \leq T \leq T_3 \quad (\beta_1 > 0) \\ \beta_2(T - T_2) & \text{for } T_3 \leq T \leq T_2 \quad (\beta_2 < 0) \\ 0 & \text{for } T < T_1 \text{ and } T > T_2. \end{cases}$$

Let $T(x)$ take the value T_3 when $x = l < 0$. Then for the interval $(l, 0)$ the solution is given by the equation

$$\lambda d_2T/dx^2 + udT/dx + \beta_1(T - T_1) = 0. \tag{1.5}$$

In the integration of this equation it must be borne in mind that if $T_0 = T_1$, then $u = 2(\lambda\beta_1)^{1/2}$; according to [12], and hence, for $T_0 < T_1$, $u < 2(\lambda\beta_1)^{1/2}$. The solution has the form

$$T|_{x \in [l, 0]} = C_1 \exp(-ux/2\lambda) \sin^{1/2}\lambda^{-1} \sqrt{4\lambda\beta_1 - u^2x} + T_1. \tag{1.6}$$

The constant C_1 is determined from the condition $T|_{x=l} = T_3$:

$$C_1 = \frac{(T_3 - T_1) \exp(ul/2\lambda)}{\sin^{1/2}\lambda^{-1} \sqrt{4\lambda\beta_1 - u^2l}}. \tag{1.7}$$

For $x \leq l$ the solution is given by Eq. (1.1) in which $F(T) = \beta_2(T - T_2)$. This solution has the form

$$\begin{aligned} T|_{x \leq l} &= C_2 \exp(r_2x) + T_2, \\ (r_2 &= -u/2\lambda + \sqrt{u^2/4\lambda^2 + |\beta_2|/\lambda}, \\ C_2 &= (T_3 - T_2) \exp(-r_2l). \end{aligned}$$

When $x = 0$ and $x = l$ the conditions of equality of the first derivatives must be satisfied. This gives us two equations for the determination of l and u

$$-(T_1 - T_0)u = \frac{1}{2} \frac{(T_3 - T_1) \exp(ul/2\lambda) \sqrt{4\lambda\beta_1 - u^2}}{\sin^{1/2}\lambda^{-1} \sqrt{4\lambda\beta_1 - u^2l}}, \tag{1.8}$$

$$(T_3 - T_2) r_2 = \left[\frac{-u}{2\lambda} \sin \left(\frac{1}{2} \lambda^{-1} \sqrt{4\lambda\beta_1 - u^2} l \right) + \right. \\ \left. + \cos \left(\frac{1}{2\lambda} \sqrt{4\lambda\beta_1 - u^2} l \right) \times \right. \\ \left. \times \frac{1}{2\lambda} \sqrt{4\lambda\beta_1 - u^2} \right] \frac{(T_3 - T_1)}{\sin \left(\frac{1}{2} \lambda^{-1} \sqrt{4\lambda\beta_1 - u^2} l \right)}. \quad (1.9)$$

This system, however, is unsuitable for solution and investigation. Since T_3 is usually close to T_2 , we convert to the limit $T_3 \rightarrow T_2$. This limiting transition can be interpreted as replacement of the function $F(T)$ in the interval $[T_1, T_2]$ by the function $\beta(T - T_1)$, so that the area of the corresponding triangle is equal to J . In this case we have

$$\beta = 2J / (T_2 - T_1)^2.$$

From (1.9) we obtain

$$\operatorname{tg} \left(\frac{1}{2} \lambda^{-1} \sqrt{4\lambda\beta - u^2} l \right) = u^{-1} \sqrt{4\lambda\beta - u^2}. \quad (1.10)$$

Then (1.8) takes the form

$$u \exp(-ul/\lambda) = \sqrt{2\lambda J} / T_1 - T_0. \quad (1.11)$$

It should be borne in mind here that for a prescribed u a solution of (1.10) given by the first negative root is considered. System (1.10), (1.11) uniquely determines l and u . For $u \rightarrow 0$ we have $l \sim \pi(\lambda/\beta)^{1/2}/2$ and $l \sim 2\pi\lambda/(4\lambda\beta - u^2)^{1/2}$ as $u \rightarrow 2(\lambda\beta)^{1/2}$. An approximate expression for l is

$$l \approx -2\pi\lambda / \sqrt{4\lambda\beta - u^2} + \pi/2 \sqrt{\lambda/\beta}, \\ u \rightarrow 0 \quad \text{as } T_0 \rightarrow -\infty, \\ u \rightarrow 2\sqrt{\lambda\beta} \quad \text{as } T_0 \rightarrow T_1. \quad (1.12)$$

For small u we have $\exp(-ul/\lambda) \approx 1$ and formula (1.11) becomes formula (1.3). Since $l < 0$, formula (1.11) gives a value of u less than that given by (1.3).

Thus, to calculate u we must calculate the integral J and then solve the system (1.10), (1.11). The required value of u can be "tracked down" fairly rapidly when one considers that its maximum possible value is $2(\lambda\beta)^{1/2}$. After finding l and u we obtain the temperature distribution

$$T|_{x \geq 0} = (T_1 - T_0) \exp(-ux/\lambda) + T_1, \\ T|_{l \leq x \leq 0} = c \exp(-\frac{1}{2}ux/\lambda) \sin \left(\frac{1}{2} \lambda^{-1} \sqrt{4\lambda\beta - u^2} x \right) + T_1, \\ T|_{x \leq -l} = T_2 \quad c = -2(T_2 - T_1) \exp(ul/\lambda) \sqrt{\lambda\beta/4\lambda\beta - u^2}.$$

The difficulty arising out of introduction of the ignition temperature T_1 has been noted in many references. It is difficult to determine this temperature experimentally, but it must come into theoretical models, since usually there is a range of temperatures greater than T_0 at which the gas does not react. If the Arrhenius law is used for the reaction rate $F(T) = \exp(-E/RT)(A - BT)$,

In this case the value of T_1 can be chosen so that after T_1 the function $F(T)$ begins to increase rapidly. Some arbitrariness in the choice of T_1 will not be very significant in this case.

In [6, 10] the following method was used to eliminate the ignition temperature. In formula (1.3) the lower limit T_1 of the integral is replaced by T_0 , and the difference $T_1 - T_0$ by the difference $T_2 - T_0$. While replacement of the lower limit is quite valid, since in the interval $[T_0, T_1]$ function $F(T)$ is close to zero, there appear to be no grounds for the substitution of $T_2 - T_0$, if T_0 differs greatly from T_1 . For illustration and comparison we consider an example from [9], for the case of interest to us, i. e., equality of the thermal diffusivity and the diffusion coefficient (in the notation of [9] the case $\alpha = 1$). Function

$$F(T) = 10^4 \exp(-15000/T)(2300 - T), \quad \lambda = 1, \\ T_0 = 300, T_2 = 2300, \quad F(1000) \approx 0, F(1100) \approx 1.6, \\ F(1200) \approx 3.9, F(1300) \approx 99, F(1400) \approx 202.$$

We put $T_1 = 1200$; then

$$T_1 - T_0 = 900, T_2 - T_0 = 2000; J = 898 \cdot 10^3.$$

If we use formula (1.3), we obtain $u = 1.5$. If we replace $T_1 - T_0$ by $T_2 - T_0$, we obtain $u = 0.67$. The exact value of u , found in [9] by numerical integration, was 0.71. We calculate u by the method proposed in the present paper. We have $\beta = 1.48$ and omitting the intermediate trial steps, we put $u = 0.60$. Then from (1.10) we have $l \approx -1.6$, $u \exp(-ul) = 1.56$. The right side of (1.11) is 1.5 and, hence, u can be taken as 0.60. If we take $T_1 = 1100$ or $T_1 = 1300$, we obtain approximately the same value of u .

§2. Combustion of condensed substances. The same method can be used to investigate the combustion of condensed substances (powders and solid rocket fuels). Let the solid phase (k -phase) occupy the region $x > 0$. We choose the origin of coordinates on the surface of combustion of the k -phase and, hence, the solid fuel moves with velocity u toward the surface $x = 0$. On the surface $x = 0$ the k -phase is decomposed and in the region $x < 0$ there are gaseous combustion products leaving the surface with velocity αu , where $\alpha = \rho_1/\rho_2$, and ρ_1, ρ_2 are the densities of the k -phase and the gas, respectively. The decomposition of the k -phase can be endothermic, exothermic, or thermoneutral. We will assume that heat uptake or heat release in the k -phase depends on q ; $q > 0$ in the case of endothermic decomposition, $q < 0$ in the case of exothermic decomposition, and $q = 0$ in the case of thermoneutral decomposition. Then

$$\lambda_1 d^2T/dx^2 + u dT/dx = 0, \quad T|_{x=0} = T_1, \\ T|_{x \rightarrow +\infty} = T_0 \quad (x \geq 0), \\ \lambda_2 d^2T/dx^2 + \alpha u dT/dx + F(T) = 0, \\ T|_{x \rightarrow -\infty} = T_2, \quad T|_{x=0} = T_1 \quad (x \leq 0),$$

and also

$$k_1 dT/dx|_{x=+0} - k_2 dT/dx|_{x=-0} = q\rho_1 u,$$

where k_1 and k_2 are the thermal conductivities of the k -phase and gas, respectively, and c_1 and c_2 are the corresponding specific heats.

To solve this problem we proceed as in §1, by linearizing $F(T)$ in the interval $[T_1, T_2]$. Omitting similar calculations, we write the system for l and u

$$\operatorname{tg} \left(\frac{1}{2} \lambda_2^{-1} \sqrt{4\lambda_2\beta - \alpha^2 u^2} l \right) = (\alpha u)^{-1} \sqrt{4\lambda_2\beta - \alpha^2 u^2}, \quad (2.1)$$

$$\frac{k_2 \lambda_2^{-1} \sqrt{2\lambda_2 J}}{k_1 \lambda_1^{-1} (T_1 - T_0) + q} = u \exp \left(\frac{-\alpha u l}{\lambda_2} \right), \quad (2.2)$$

$$l \approx -\frac{2\pi\lambda_2}{\sqrt{4\lambda_2\beta - \alpha^2 u^2}} + \frac{1}{2} \pi \left(\frac{\lambda_2}{\beta} \right)^{1/2}. \quad (2.3)$$

Relationships (2.1) and (2.2) give u as a function of T_0 . If $q > 0$ (endothermic decomposition of k -phase), then when $T_0 = T_1$ the velocity does not attain the value $u = 2(\lambda_2\beta)^{1/2}/\alpha$. In the case $q = 0$ the situation is similar to that considered in §1. If $q = -p < 0$, then at the maximum permissible value of T_0 , given by the relationship

$$k_1 \lambda_1^{-1} (T_1 - T_0) = p\rho_1, \quad \text{or} \quad C_1 (T_1 - T_0) = p, \quad (2.4)$$

the velocity takes the value $u = 2(\lambda_2\beta)^{1/2}/\alpha$. We note that the denominator on the left side of (2.2) cannot be negative, since this would mean that $p > C_1(T_1 - T_0)$ and the process depends on the decomposition of the k -phase, and not on the reaction in the gas.

§3. Behavior of temperature gradient at $x = 0$. We use the preceding results to investigate the behavior of the gradient at $x = 0$. The absolute value of the gradient will be considered. In the case of combustion of a gas we have from (1.11)

$$\varphi = (T_1 - T_0) u / \lambda = \lambda^{-1} \sqrt{2\lambda J} \exp(ul/\lambda), \\ \varphi \rightarrow \sqrt{2J/\lambda} \quad \text{as } T_0 \rightarrow -\infty, \quad u \rightarrow 0; \\ \varphi \rightarrow 0 \quad \text{as } T_0 \rightarrow T_1. \quad (3.1)$$

It is clear from (3.1) that φ is a decreasing function of $u(T_0)$ and has no turning points. The greatest value of φ is $(2J/\lambda_2)^{1/2}$ and is reached as $T_0 \rightarrow -\infty$. For each possible value of φ there is one combustion regime.

In the case of combustion of condensed substances we obtain from formula (2.2)

$$\varphi = \frac{(T_1 - T_0) u}{\lambda_1} = \frac{1}{k_1} \left[\frac{k_2}{\lambda_2} \sqrt{2\lambda_2 J} \exp \frac{\alpha u l}{\lambda_2} - q \rho_1 u \right]. \quad (3.2)$$

Relationships (1.8), (1.10), and (3.2), (2.1) give φ as a function of u and, hence, as a function of T_0 . These relationships can also give u as a function of φ .

If $q \geq 0$ we proceed in a similar way: if $T_0 \rightarrow -\infty$, then $\varphi \rightarrow k_2 k_1^{-1} \cdot (2J/\lambda_2)^{1/2}$ — the greatest value of the gradient. As $T_0 \rightarrow T_1$ the value of $\varphi \rightarrow 0$; φ is a decreasing function of T_0 and for each permissible value of φ there is one combustion regime.

We consider the case $q < 0$. Then ($q = -p < 0$)

$$\begin{aligned} \varphi &\rightarrow k_2 k_1^{-1} \sqrt{2J/\lambda_2} \quad \text{as } T_0 \rightarrow -\infty, u \rightarrow 0, \\ \varphi &\rightarrow 2k_1^{-1} \sqrt{\lambda_2 \beta} \rho_2 p \\ \text{as } k_1 \lambda_1^{-1} (T_1 - T_0) &\rightarrow p \rho_1 (c_1 (T_1 - T_0) \rightarrow p), \\ u &\rightarrow 2\alpha^{-1} \sqrt{\lambda_2 J}. \end{aligned}$$

It is obvious that we can regard $p < c_2(T_2 - T_1)$. Hence

$$\varphi < 2k_2 k_1^{-1} \sqrt{2J/\lambda_2} \quad \text{as } u \rightarrow 2\alpha^{-1} \sqrt{\lambda_2 \beta}.$$

We find $d\varphi/du$ (in view of the fact that $du/dT_0 > 0$, the sign of $d\varphi/du$ is the same as that of $d\varphi/dT_0$):

$$\frac{d\varphi}{du} = \frac{1}{k_1} \left[\frac{k_2}{\lambda_2} \sqrt{2\lambda_2 J} \exp \frac{\alpha u l}{\lambda_2} \frac{\alpha}{\lambda_2} (ul) + p \rho_1 \right].$$

It is easy to see that $d\varphi/du \rightarrow p \rho_1 > 0$ as $u \rightarrow 2(\lambda_2 \beta)^{1/2}/\alpha$; as $T_0 \rightarrow -\infty$,

$$\begin{aligned} \frac{d\varphi}{du} &\rightarrow \frac{1}{k_1} \left[-\frac{k_2}{\lambda_2} \sqrt{2\lambda_2 J} \frac{\alpha}{\lambda_2} \frac{\pi}{2} \left(\frac{\lambda_2}{\beta} \right)^{1/2} + p \rho_1 \right] = \\ &= \frac{1}{k_1} \left[p - \frac{1}{2} \pi c_2 (T_2 - T_1) \right] < 0. \end{aligned}$$

Hence, there is a point at which $d\varphi/du = 0$, but this will be a minimum, and not a maximum, point of the gradient. The question arises as to whether there are other turning points. It is obvious that for specific values of the parameters we can use (3.2), (2.1) to construct the graph of the function $\varphi(u)$ and verify the presence of a maximum. For small p there will be no other turning points. The rapid reduction of the factor $\exp(\alpha ul/\lambda_2)$ with increase in u suggests that, apart from the indicated minimum, there will be no other turning points for any p .

54. Application to investigation of the stability of combustion. As was mentioned in the introduction, there have been many investigations of the stability of powder combustion [1–5, 13]. It was suggested in [1, 2] that there is a value of the gradient φ^* such that a steady-state regime with a gradient greater than φ^* is impossible. The results of the present paper confirm the presence of a largest gradient for steady-state regimes. However, in the theory of stability of powder combustion it is very important to find out if this largest value is the maximum.

It was suggested in [2] that there is a maximum and that when $d\varphi/dT_0 < 0$ the regime is stable, and when $d\varphi/dT_0 > 0$ it is unstable. A very general investigation of stability was made in [5]. Since in our model, as in [1, 2, 13], the temperature of the combustion surface is regarded as constant, we use the results of [5] for this case. It was shown in [5] that if

$$k = (T_1 - T_0) d \ln u / dT_0 < 1,$$

then combustion is stable and, if $k > 1$, then it is unstable. It is easy to see that the condition $k < 1$ (> 1) is equivalent to the condition $d\varphi/dT_0 < 0$ (> 0). But, as was shown above, in the case of endothermic decomposition of the k -phase (such a case is considered in [1, 2]), k is always less than 1, i. e., in this case the steady-state regime is always stable. This result seems quite natural, since the considered model of powder combustion is similar to the model of flame propagation, in which the steady-state regime is always stable [7]. We note incidentally that in the case of normal flame propagation $k < 1$ and, hence, stability will ensue.

In the case of exothermic decomposition we obtain the following picture. Here there is a minimum of $\varphi(T_0)$ and, hence, for small T_0 we obtain $d\varphi/dT_0 < 0$, consequently, stability. For large T_0 we have $d\varphi/dT_0 > 0$ and instability of the corresponding regimes. It is obvious, however, that this will not be instability due to decay of the process but, on the contrary, instability due to acceleration of the combustion process.

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