ESTABLISHMENT OF STEADY FLAME PROPAGATION
WHEN IGNITING A GAS BY A HEATED SURFACE

A. G. Merzhanov, B. I. Khaikin,
and K. G. Shkadinskii

Steady-state combustion is preceded by an essentially unsteady process encompassing the time interval from the initiation of the action of the external heat source to the establishment of the stationary front propagation velocity. In studies of the ignition of condensed and gaseous systems ([1-3] and others) the unsteady process was studied for regimes having a very marked inductive nature, although only to the instant of sharp temperature rise. The subsequent course of the process, culminating with transition to steady-state combustion, and also the regimes which do not have an inductive nature of initiation of the chemical reactions, have not been examined, since in the gas case this involves major difficulties even when using an electronic computer, while in the case of condensed substances there is also some confusion in the physical formulation of the problem. In the present paper we use several simplifing assumptions to study the process of transition to the steady-state combustion regime with thermal initiation of the chemical reaction in a combustible gas by a heated surface. The essence of the article are the conclusions drawn on the basis of numerical computer calculations.

PROBLEM FORMULATION

At the initial time a gas capable of exothermal transformation with the temperature T_0 is brought into contact with a hot wall whose temperature is T_W $(T_0 < T_W)$.

We assume that the wall temperature does not change in time. The process may be described by the system of differential equations

$$\rho_t' + (\rho v)_x' = 0, \qquad R\rho T \left[(1 - \eta) / \mu_1 + \eta / \mu_2\right] = p_0$$
$$c_p\rho \left(T_t' + vT_x'\right) = (\lambda T_x')_x' + Q\rho (1 - \eta) k \exp\left(-E / RT\right) \qquad (1)$$
$$\rho \left(\eta_t' + v\eta_x'\right) = (D\rho\eta_x')_x' + \rho (1 - \eta) k \exp\left(-E / RT\right)$$

where

$$p_0 = R\rho_0 T_0 / \mu_1, \qquad \lambda = \lambda_0 (T / T_0)^s, \qquad D = D_0 (\rho_0 / \rho) (T / T_0)^s$$

with the initial and boundary conditions

$$T = T_0, \quad v = 0, \quad \eta = 0, \quad \rho = \rho_0 \ \text{for} \ t = 0$$
$$T = T_w, \quad v = 0, \ \eta_x' = 0 \qquad \qquad \text{for} \ x = 0$$

Here ρ = density, v = gas velocity, T = temperature, c_p = specific heat, Q = thermal effect per unit mass of the combustible gas mixture, η = conversion efficiency (relative weight concentration of the combustion products), k = pre-exponent, E = activation energy, R = gas constant, μ_1, μ_2 = molecular weights, p_0 = pressure, λ = thermal conductivity, D = diffusivity.

The system (1) consists of the equations of continuity, heat conduction, diffusion, and the equation of state of the mixture of two ideal gases. We examine the case of first-order reaction. Equations (1) are written on the following assumptions: a) the velocity caused by chemical conversions and thermal expansion is significantly less than the speed of sound and, consequently, the pressure may be considered constant and the work of compression may be neglected in the energy equation; b) there is not free convection; c) the specific heat and thermal conductivity do not depend on the composition.
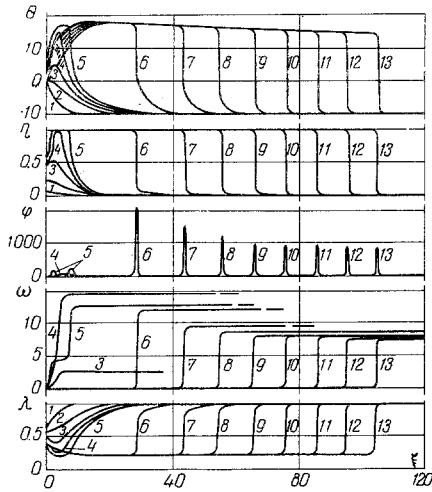
Fig. 1

The entire transient process (whose time we denote by t_0) can be divided into two stages: the process of nonstationary front formation (t_1) and the process of nonstationary front propagation (t_2), terminating with the onset of stationary combustion $(t_0 = t_1 + t_2)$. Because of the asymptotic nature of the transient process, this division is arbitrary. The nonstionary combustion front may be considered formed if at any point of the mixture the conversion efficiency becomes close to one. Similarly, the front may be considered established if its velocity is nearly stationary. For definiteness, in the following we assume that the nonstationary front is formed if at any point of the mixture η becomes equal to 0.9, and that the front is established if the value of the nonstationary velocity of the front differs from its stationary value by 10%. Other conditions for the selection of t_1 and t_2 alter only their magnitude, without introducing any significant changes in the final results.

In the following the analysis of the transient process will be made with the aid of dimensionless space–time quantities, for which the dimensionless variables and parameters are

$$\tau = \frac{t}{t_*}, \qquad t_* = \frac{c_p RT_*^2}{EQk} \exp \frac{E}{RT_*}, \qquad \xi = x\left(\frac{c_p \rho_0}{\lambda_* t_*}\right)^{1/2}$$

$$\omega = v\left(\frac{c_p \rho_0 t_*}{\lambda_*}\right)^{1/2}, \qquad \theta = \frac{(T - T_*)E}{RT_*^2}, \qquad \theta_w = \frac{(T_w - T_*)E}{RT_*^2}$$

$$\theta_0 = \frac{(T_* - T_0)E}{RT_*^2}, \qquad \gamma = \frac{c_p RT_*^2}{EQ}, \qquad z = \frac{(T_w - T_0)c_p}{Q}$$

$$\chi = \rho/\rho_0, \quad \beta = RT_*/E, \quad \sigma = \mu_2/\mu_1, \quad L = c_p D_* \rho_*/\lambda_*, \quad \varphi = (1 - \eta)\exp\frac{\theta}{1 + \beta\theta}, \qquad m = \int_0^\xi \chi\, d\xi$$

where T_* is a scale temperature, whose choice will be indicated later (the asterisk indicates that the value of the given parameter is referred to the temperature T_*).

According to [2] the initiation of chemical reaction in a combustible substance by heat coming from a wall takes place qualitatively differently for different values of the parameter z. Accordingly, the entire transient process, whose various regimes will be examined below, will take place differently, depending on the value of z.

Inductive Ignition Mode. This mode is realized in those cases in which the wall temperature T_w is significantly lower than the stationary combustion temperature $T_b = T_0 + Q/c_p$ (the quantity z is less than 0.5-0.7). For this regime it is convenient in the calculations to take the wall temperature T_w ($\theta_w = 0$, $z = \gamma\theta_0$) as the scale temperature T_*. The space–time pattern of the inductive ignition regime is shown in Fig. 1 for the following values of the parameters: $\theta_0 = 10$, $\gamma = 0.04$, $\beta = 0.03$, $\sigma = 0.5$, $s = 0.6$; the numerals 1, . . . , 13 in the figure correspond to the following times:

	1	2	3	4	5	6	7
$\tau =$	4.1	38.3	48	48.2	48.3	49.3	50.3
	8	9	10	11	12	13	
$\tau =$	51.3	52.3	53.3	54.3	55.3	56.3	

The process taking place during the time t_1 has been described in detail, and here we examine only the process taking place during the time interval t_2 (in this case the time introduced for formation of the nonstationary front practically coincides with the ignition delay time found in [2]).

As a result of the marked acceleration of the chemical reaction at times close to t_1, the temperature peak previously formed at some distance from the wall very rapidly reaches its maximal value, exceeding the mixture stationary combustion temperature T_b (Fig. 1). Further increase of the temperature peak is terminated as a result of complete burnup of the combustible mixture in the narrow zone near the temperature peak. Beyond the limits of this narrow zone the conversion efficiency still remains everywhere small. After this the region of high conversion efficiency and high temperature begins to propagate in both directions and two fronts are formed.
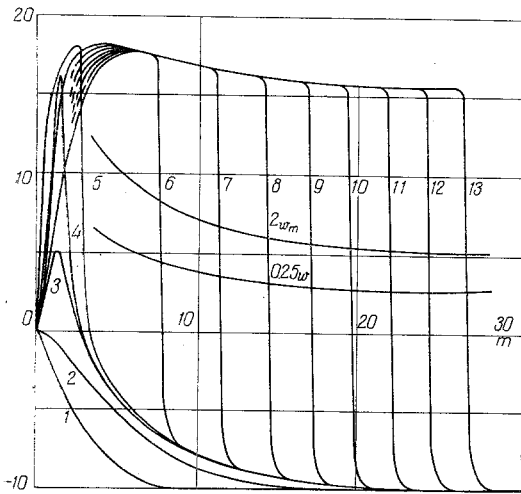
Fig. 2

One of these fronts travels toward the wall until the unreacted combustible mixture located between the temperature peak point and the wall burns up. The other front propagates away from the wall in the direction of the fresh unreacted mixture. The rate of propagation of this front decreases in the course of time, approaching a constant value — the stationary flame propagation velocity. The resulting temperature peak causes marked expansion of the gas. The graph for the gas velocity immediately after occurrence of the maximal temperature has two "steps" which correspond to the two propagation fronts. After burnup of the gas near the wall one step disappears, and thereafter as a result of cooling of the hot combustion products by the cooler wall the velocity in the region between the wall and the combustion front propagating into the fresh mixture acquires small negative values, decreasing in absolute magnitude as the combustion front moves farther away.

To evaluate the time t_2 it is advisable to examine the space—time pattern of the course of the process in the Lagrangian (mass) coordinate system; specifically we take the quantity m as the independent variable in place of the coordinate ξ. Figure 2 shows the temperature distribution in these coordinates for the following values of the parameters: $\theta_0 = 10$, $\gamma = 0.04$, $\beta = 0.03$, $s = 0.6$, $\sigma = 0.5$; the numerals 1, . . . , 13 in the figure correspond to the following times:

	1	2	3	4	5	6	7
$\tau =$	4.1	38.3	48	48.2	48.3	49.3	50.3

	8	9	10	11	12	13
$\tau = $	51.3	52.3	53.3	54.3	55.3	56.3

Also shown here are the values of the dimensionless front linear velocity w (velocity relative to the wall) and the dimensionless front mass velocity w_m at times corresponding to frontal passage through the plane with coordinate m.

We see from Fig. 2 that nonstationary front propagation does not alter significantly the temperature distribution ahead of the front, which forms at the moment $t = t_1$, and the stationary velocity is nearly reached when the gas mass heated during the time t_1 burns up.

The magnitude of the heated gas mass can be found approximately by solving the heat conduction equation in Lagrangian coordinates for semi—infinite space [4]

$$M \approx 2 \sqrt{\lambda_0 \rho_0 t_1 / c_p} \tag{2}$$

where λ_0 is the thermal conductivity for $T = T_0$. To calculate the time t_2 we should divide the quantity M by the average value of the unsteady mass velocity u during this time. However we see from Fig. 2 that this velocity does not differ markedly from the stationary front propagation mass velocity u_0, and therefore the following formula is valid for the approximate estimate of the time t_2:

$$t_2 \approx \frac{2}{u_0} \left(\frac{\lambda_0 \rho_0 t_1}{c_p} \right)^{1/2} \tag{3}$$

The value of t_1 in (3) can be estimated on the basis of the results of [2], and the value of u_0 can be found with the aid of the Zel'dovich—Frank-Kamenetskii formula [5].

We transform (3) to a different form, introducing the characteristic stationary combustion time

$$t_b = \frac{\lambda_b \rho_b}{c_p u_0^2} \tag{4}$$

where λ_b, ρ_b are the thermal conductivity and density of the combustion products for $T = T_b$. The meaning of the quantity t_b is the time for burnup of the heated layer for stationary combustion. Excluding u_0 from
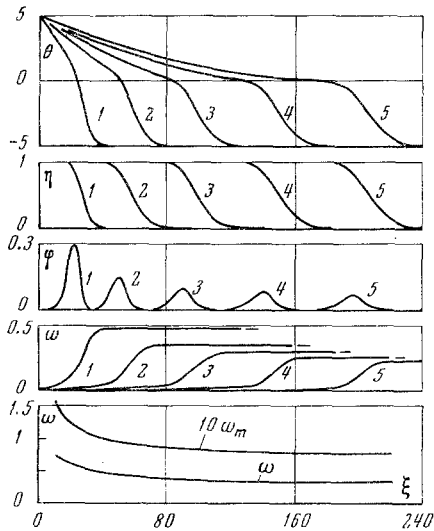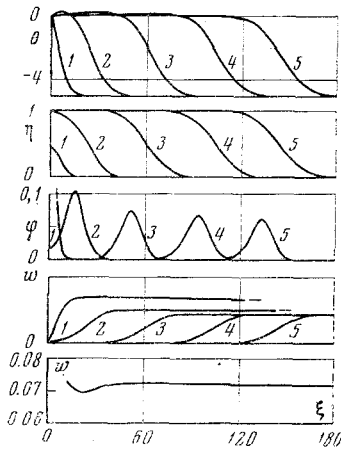
Fig. 3

Fig. 4

(3), we find the connection between the times characterizing all stages of the process — ignition, nonstationary combustion, and stationary combustion:

$$t_2 \approx 2\sqrt{\lambda_0\rho_0/\lambda_b\rho_b}\ \sqrt{t_1 t_b} \qquad (5)$$

The factor preceding the quantity $\sqrt{t_1 t_b}$ is usually of order one and, consequently, t_2 is of order $\sqrt{t_1 t_b}$. As is known, the quantity t_1 is proportional to $\exp (E/RT_0)$ and the quantity t_0 is proportional to $\exp (E/RT_b)$. Thus, in the nondegenerate ignition mode $t_1 > t_2 > t_b$, and the entire time t_0 for the nonstationary process of transition to the stationary combustion regime actually coincides with the ignition time t_1. This relationship between the times is the characteristic feature of the nondegenerate ignition regime. If the wall temperature T_W is increased while maintaining the other conditions constant, then the time t_2 decreases considerably more slowly than does the time t_1, and for some values of the wall temperature $T_W (T_W < T_b)$ the time t_1 becomes equal to t_2. However this temperature now corresponds to the so-called "intermediate" regime, having a different nature of the course of the process, and the formulas for t_1 and t_2 become invalid.

Ignition Mode. This mode is realized when the wall temperature T_W exceeds considerably the stationary T_b temperature burning (the value of z is more than 1.7–2). For this mode it is convenient to take $T_b (\theta_0 = 1/\gamma)$ as the scale temperature in the calculation.

The space–time pattern of the course of the process is shown in Fig. 3 for the following values of the parameters: $\theta_0 = 5$, $\theta_W = 5$, $\gamma = 0.2$, $\beta = 0.1$, $\sigma = 0.5$, s = 0.6; the numerals 1, . . . , 5 in the figure correspond to the following times:

$$\tau = \begin{matrix} 1 & 2 & 3 & 4 & 5 \\ 32 & 94 & 196 & 340 & 505 \end{matrix}$$

Also shown here are the values of the dimensionless apparent and mass velocities of the front at times corresponding to frontal passage through the plane with the coordinate ξ. In constrast with the inductive ignition mode in the ignition mode there is no lengthy process of heating of the mixture, in the mixture, in the course of which the conversion efficiency is everywhere very small (there is no so-called ignition delay). In this mode the conversion efficiency near the surface ignition delay). In this mode the conversion efficiency near the surface becomes close to one practically instantaneously, i.e., the nonstationary front formation time t_1 is small, and the total transient process time t_0 essentially coincides with the nonstationary burning time t_2.

In contrast with the ignition mode, in the mode in question here there is no spatial temperature peak and there is always only a single chemical reaction propagation front, directed away from the wall. Accordingly, there is always only a single velocity "step," caused by motion of the fresh mixture as a result of thermal expansion and change of the molecular weight of the gas in the burning zone.

The nonstationarity of the front propagation process in the ignition mode is due to the presence of thermal flux from the hot wall into the burning zone. As the front moves away from the wall the heat flux into the burning zone decreases and the front velocity approaches its stationary value. The front may be considered established when the thermal flux from the wall into the burning zone becomes small in comparison with the heat released as a result of chemical reaction. This makes it possible to estimate the magnitude of the nonstationary burning time t_2 (and, therefore, t_0). The heat flux from the wall into the burning zone for times close to t_2 can be established approximately by solving in Lagrangian coordinates the problem of wall heating by the combustion products

$$q = (T_w - T_b)\left(\frac{c_p \lambda_b \rho_b}{\pi t_2}\right)^{1/2}\exp\left(-\frac{c_p M^2}{4\lambda_b \rho_b t_2}\right) \qquad (6)$$
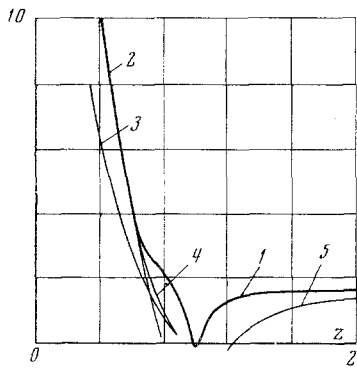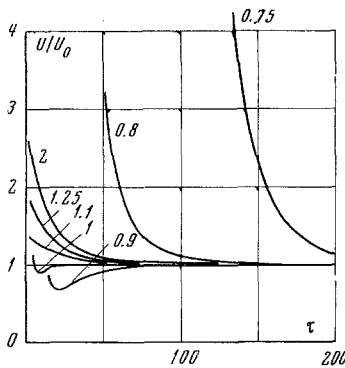
Fig. 5

Fig. 6

where q is the heat flux from the wall into the burning zone, and M is the mass of the burned gas at the time t_2. The values of M can be taken approximately equal to the product of the stationary mass burning velocity u_0 by the time (M $\approx u_0 t_2$). Assuming the flux from the wall into the burning zone small in comparison with the heat release rate owing to chemical reaction (for definiteness, q = 0.1 Qu_0), we can obtain the approximate formula for t_2:

$$\sqrt{t_2 / t_b} \; \exp \; (t_2 / 4t_b) \; = (10 / \sqrt{\pi}) \; (T_w - T_b) / (T_b - T_0) \qquad (7)$$

where t_b is defined by (4).

If we increase the wall temperature T_W while maintaining the other conditions unchanged, in accordance with (7) the transient process time t_0 ($t_0 \approx t_2$) in the ignition mode increases, when in the induction ignition mode it decreased. Therefore in the mode which is intermediate between these two limiting modes the quantity t_0 has a minimum as a function of the wall temperature.

Intermediate Mode. This mode is realized in those cases in which the wall temperature T_W is close to the burning temperature T_b (z is close to one). It is difficult to indicate sharp boundaries between the extreme and intermediate regimes and the intermediate mode can be considered to be "degenerate" in the sense that as the wall temperature approaches the burning temperature from both higher and lower temperatures the properties of one limiting mode are gradually lost and those of the other limiting mode are gradually acquired.

For example, if the wall temperature is increased to bring it close to the burning temperature, then in comparison with the induction ignition mode the preheating stage begins to be characterized by increasingly higher conversion efficiencies, the temperature peak becomes increasingly smaller and shifts toward the wall. The chemical reaction front directed toward the wall becomes increasingly less marked and gradually disappears, the fraction of the time t_1 in the overall time t_0 decreases, and the fraction of the time t_2 increases. However, if we reduce the wall temperature, bringing it close to the burning temperature, then there is "degeneration" of the ignition mode. In this case the wall influence on the nonstationary chemical reaction front propagation process diminishes and at some temperature close to the burning temperature there appears a small temperature peak in space. The time t_1 increases and t_2 decreases.

The greatest degree of degeneration of the two limiting modes is achieved when the wall temperature equals the burning temperature. Figure 4 shows the space-time pattern of the course of the process for the following values of the parameters: $\theta_0 = 5$, $\gamma = 0.2$, $\beta = 0.1$, s = 0.6, $\sigma = 0.5$; the numerals 1, ..., 5 correspond to the following times:

$$\tau = \begin{matrix} 1 \\ 14.5 \end{matrix} \quad \begin{matrix} 2 \\ 71 \end{matrix} \quad \begin{matrix} 3 \\ 199 \end{matrix} \quad \begin{matrix} 4 \\ 344 \end{matrix} \quad \begin{matrix} 5 \\ 481 \end{matrix}$$

Here the temperature T_b is taken as the scale temperature T_*. We see from the figure, specifically, that a practically stationary burning front can form even at distances from the wall of the order of the thickness of the preheated layer for stationary combustion. The numerical calculations for different values of the parameters show that the time t_0 for $T_W = T_b$ is close to the value of t_b found from (4) (t_0 amounts to 0.5-1 times t_b).

Figure 5 shows the logarithm of the ratio of the nonstationary process total time t_0 to t_b (ln t_0/t_b) versus z (curve 1). As we would expect, a minimum of t_0 occurs for $T_W = T_b$. This figure also shows the values of ln (t_1/t_b) (curve 2, t_1 calculated using the formula of [2]), ln (t_2/t_b) (curve 3, t_2 calculated using (5), u_0 calculated using the formula of [5]), ln ($t_1 + t_2$)/t_b (curve 4), and ln (t_2/t_b) (curve 5, t_2 calculated using (7)). We see from the figure that the approximate formulas agree quite well with the numerical calculations in those regions where the approximations used in obtaining these formulas are valid.

Figure 6 shows for the following values of the parameters: $\theta_0 = 14.7$, $\gamma = 0.047$, $\beta = 0.05$, $\sigma = 1$, $s = 0.6$, the ratio of the mass nonstationary burning velocity u to its stationary value u_0 versus dimensionless time τ ($T* = 0.75\ T_b$) for various values of the wall temperature (the numerals indicate the values of z). The abscissa coordinate of each curve corresponds to the front formation time. We see from the figure that the nonstationary burning velocity is higher than the stationary value, and the highest value of the nonstationary velocity for different values of the wall temperature decreases as the wall temperature approaches the burning temperature from both higher and lower temperatures. In this region the nonstationary burning velocity approaches the stationary value from lower values. Analysis of the space-time distribution showed that the reason for this is the influence of the relatively cold wall and the burning front which forms near the wall.

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