STUDY OF THE EXTINCTION OF GUNPOWDER IN THE COMBUSTION MODEL WITH A VARIABLE SURFACE TEMPERATURE

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The results of a calculation of the rate of transient combustion of gunpowder during a fall in pressure are presented; these are obtained by the numerical integration of the equations of transient-combustion theory, allowing for the variable surface temperature of the k phase. For rapid and severe pressure drops extinction always occurs, no introduction of special extinction conditions being required. The change in the rate of burning during the extinction process is of a smooth nature.

It is already well known from experimental data that gunpowder is extinguished when the pressure falls rapidly and fairly severely [1]. In order to study the extinction of gunpowder we shall here use the theory of transient combustion of Ya. B. Zel'dovich and B. V. Novozhilov [2-4]. The basic assumptions of this theory are as follows:

1) The chemical reactions in the k phase only take place in a thin surface layer.

2) The reactive layer of the k phase and the gas flame are rearranged almost instantaneously when the external conditions alter and remain in a quasi-steady state all the time.

3) The deviation of combustion from the steady state is determined solely by the inertia of the heated layer of k phase. The rearrangement of the heated layer in a coordinate system linked to the surface of the k phase is described by the equation

$$\frac{\partial T}{\partial t} = \varkappa \frac{\partial^2 T}{\partial x^2} - u \frac{\partial T}{\partial x} \qquad (-\infty < x \leqslant 0) \tag{0.1}$$

Here x is the coordinate normal to the surface of the k phase, t is the time, $u = u(t)$ is the rate of burning, $T = T(x, t)$ is the temperature distribution in the k phase, $\varkappa$ is the thermal diffusivity of the k phase.

The thermal flux from the reaction zone into the heated layer and the surface temperature of the k phase are determined by the processes taking place in the zone of decomposition of the k phase and in the gas flame; by virtue of the assumptions made they depend solely on the instantaneous values of the pressure and rate of combustion [4]

$$(\partial T/\partial x)_{x=0} = \varphi(p, u) \tag{0.2}$$

$$T_{x=0} = T_s(p, u) \tag{0.3}$$

Equations (0.2) and (0.3) are valid in the steady-state case as well; hence, they may be determined from the experimental relationships giving the rate of steady burning and the surface temperature as functions of the pressure and initial temperature of the powder [4]. Equation (0.1), with boundary conditions (0.2) and (0.3), enables us to determine the rate of burning if the initial temperature distribution and the pressure/time law are specified.

In the case of a constant surface temperature (T_s = const), extinction occurs when it becomes impossible to match the instantaneous thermal state of the k phase to the conditions (0.2) and (0.3) [3, 5]. However,

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TABLE 1

Powder model			Pressure drop		
No. of version	k	m	No. of version	Δt	p_k
			1	1.1	0.6
			2	1.0	0.6
			3	0.02	0.85
I	1.4	10	4	2.5	0.26
			5	2.5	0.23
			6	2.0	0.37
			7	0.02	0.87
II	1.6	10			
III	1.4	15			
IV	1.4	7			
V	0.6	10			
VI	0.4	10			
VII	2	10	1	10	0.99
VIII	2	15	1	10	0.99
IX	0.5				
X	0.5	100	1	1.0	0.18

in the case of a variable surface temperature this interpretation of extinction encounters certain difficulties. The possibility of extinction taking place is introduced into the theory by assuming that the $\varphi(u)$ curves representing the (0.2) relationship for p = const contain certain limiting points corresponding to finite values of the rate of burning and temperature gradient, beyond which combustion is impossible [6, 7]. Passing out beyond these points in the process of transient combustion is considered an extinction. Both in the case of T_s = const and in the presence of limiting points, extinction takes place suddenly: Immediately before the instant of extinction the rate of burning is still quite high and in order of magnitude lies close to the rate of steady-state burning.

In this paper we shall present the results of a calculation of the rate of transient burning which occurs during a fall in pressure, allowing for the variable surface temperature of the k phase, as derived from a numerical solution of the system of equations (0.1)-(0.3). We shall show that extinction occurs even in the absence of limiting points in the relationship (0.2). The change in the rate of burning with time during the extinction process bears a smooth character.

1. Let us consider the burning of gunpowder under a variable pressure. We shall assume that up to the moment t = 0 the powder is burning steadily. It is convenient to transform to dimensionless variables

$$t' = \frac{(u^\circ)^2 t}{\varkappa}, \quad x' = \frac{u^\circ x}{\varkappa}, \quad p' = \frac{p}{p^\circ}$$
$$u' = \frac{u}{u^\circ}, \quad \varphi' = \frac{\varphi}{\varphi^\circ}, \quad T' = \frac{T - T_0}{T_s^\circ - T_0}$$

Here T_0 is the initial temperature of the powder, the "degree" superfix indicates the parameters of the original steady-state mode, the prime indicates the dimensionless variables. Subsequently the prime will be omitted, since dimensioned variables will no longer be employed. The original steady values of the dimensionless pressure, burning rate, surface temperature, and temperature gradient are equal to unity. The heat-conduction equation in dimensionless variables is

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} - u\frac{\partial T}{\partial x} \qquad (-\infty < x \leqslant 0) \tag{1.1}$$

Let us assume that the temperature and temperature gradient on the surface of the k phase are determined by the relations

$$u = p^{0.69} \exp k\,(T_s - \varphi / u) \tag{1.2}$$

$$u = e^{m(T_s - 1)} \tag{1.3}$$

Here k and m are constant quantities coinciding with the definition of [6] (m = k/r). The choice of relationships (1.2) and (1.3) signifies the choice of a particular model of powder combustion. Equation (1.2) corresponds to a constant coefficient of the temperature sensitivity of the rate of steady-state burning $\beta = (\partial \ln u^\circ / \partial T_0)_p$. Equation (1.3) approximates the law of pyrolysis of the k phase. Let us solve (1.2) and (1.3) for T_s and φ:

$$T_s = 1 + m^{-1} \ln u \tag{1.4}$$

$$\varphi = u\,[1 + (1/m - 1/k) \ln u + 0.69\, k^{-1} \ln p] \tag{1.5}$$

The isobars of Eq. (1.5) are shown in Fig. 1 for the case of k = 1.4, m = 10. For any particular pressure Eqs. (1.4) and (1.5) allow a single state of steady burning with the parameters

$$u = p^{0.69}, \quad T_s = 1 + 0.69\, m^{-1} \ln p, \quad \varphi = p^{0.69}\,(1 + 0.69\, m^{-1} \ln p) \tag{1.6}$$

(curve C in Fig. 1).

At the instant of time t = 0 a pressure drop begins, taking place in accordance with an exponential law

$$p\,(t) = p_k + (1 - p_k)\, e^{-t/\Delta t} \tag{1.7}$$

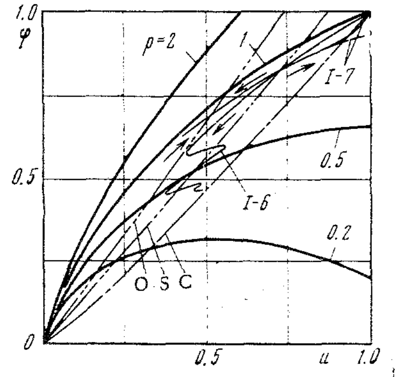

Fig. 1

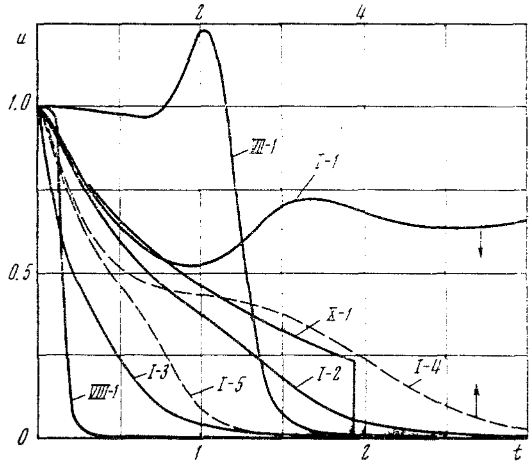

Fig. 2

Here Δt is the characteristic time of pressure drop, p_k is the pressure level after the drop.

At the initial instant of time the temperature in the k phase is distributed in accordance with the law

$$T(x, 0) = e^x \quad (-\infty < x \leqslant 0) \tag{1.8}$$

At an infinite distance from the surface the initial temperature of the powder remains intact

$$T(-\infty, t) = 0 \tag{1.9}$$

The determination of the rate of burning amounts to a solution of Eq. (1.1) subject to the conditions (1.4), (1.5), (1.7)-(1.9).

For a numerical solution of the resultant system of equations, the interval $(-\infty < x \leq 0)$ is imaged onto a unit segment $(0 \leq y \leq 1)$ by making the coordinate transformation $y = 1 - e^{\alpha x}$. Here α is the transformation parameter, selected from the point of view of securing the greatest accuracy of the numerical method, and (generally speaking) varying with time. We introduce a finite-difference approximation for the differential equation and boundary conditions in a rectangular space–time mesh (in the present case the mesh contained 32 coordinate intervals, while the time step amounted to 0.02 or under). The nonlinear algebraical system of equations arising as a result of the approximation may be solved by iteration. The rate of burning is determined at successive, discrete instants of time; the temperature distribution in the k phase is calculated at the same time.

Table 1 gives the values of the parameters k, m, Δt, p_k in the calculations, the results of which will be considered subsequently. In accordance with the table the various versions of the powder model (parameters k and m) will be denoted in the text and figures by Roman numerals, and the various versions of pressure drops (parameters Δt and p_k) by additional Arabic numerals.

2. The results of the calculations showed that there were two different modes of transient burning of the powder during a pressure drop. Figure 2 illustrates the change in the rate of burning with time for a number of the modes calculated. In version I-1 the rate of burning passes to a new steady level of $u \approx 0.7$ as time progresses, corresponding to a value of $p_k = 0.6$. This process is accompanied by fluctuations in the rate of burning; these arise during the rapid change in pressure and attenuate as the steady-state mode is approached, in agreement with [6].

In version I-2, differing slightly from I-1 simply in respect of the fall-off time, the rate of burning falls monotonically with time, reaching a value of $\sim 10^{-3}$, and becomes practically constant. Zero is never reached because of the form of Eq. (1.3), according to which, even for a surface temperature equal to the initial temperature of the powder ($T_s = 0$), the rate of burning $e^{-m} > 0$ (for $m = 10$ it amounts to $\sim 10^{-4}$). However, by comparison with the steady burning rate the new level signifies the almost complete absence of burning, and we may, therefore, consider that extinction has occurred.

The mode of slow burning so attained, despite its constant velocity, is not completely steady, by virtue of (1.6). Hence the rearrangement of the heated layer continues at a constant burning rate, and ultimately there should be an increase in the rate of combustion (a further surge) with subsequent passage to the steady condition. However, for such a slow burning rate the characteristic time for the rearrangement

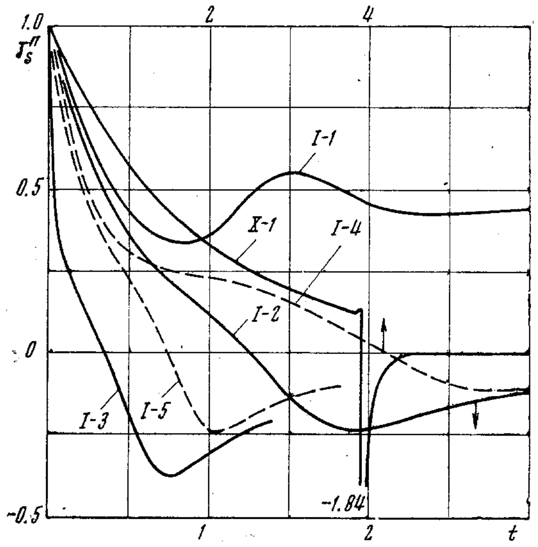

Fig. 3

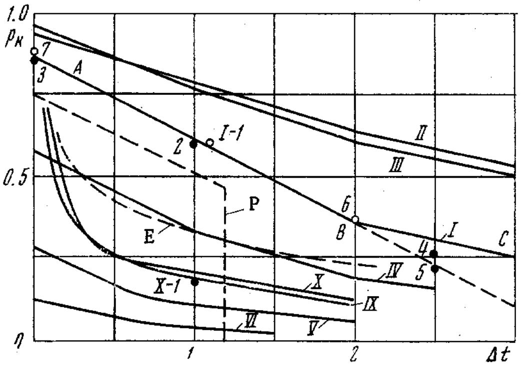

Fig. 4

of the heated layer ($\sim 1/u^2$) is extremely great, so that the transition out of the state of extinction requires extremely long intervals ($\sim 10^6$).

We shall use the term "extinction" to mean conditions of transient burning associated with a release of pressure, under which the rate of combustion does not pass out to a steady value corresponding to the new pressure level, but falls asymptotically to zero or a very small value. The remaining modes of burning may conveniently be called modes of passage to a new stationary state, or more briefly "transient modes."

3. The extinction modes obtained in the calculations are characterized by the fact that in these modes combustion does not cease abruptly but quite gradually, by virtue of a smooth and continuous reduction in combustion rate. Extinction takes place in this way even for a very rapid fall in pressure – in this case it sets in a considerable time after the completion of the pressure drop (curve I-3 in Fig. 2). The change in burning rate in both the extinction and transient modes begins in the same way for similar characteristics of the pressure drop (curves I-1 and I-2 in Fig. 2); the difference between these modes increases smoothly with the passage of time.

On analyzing the temperature distribution in the k phase obtained during the calculations, we noted that on extinction the second derivative of the temperature with respect to the coordinate at the surface of the k phase T_s'' always became negative. On the temperature profile an inflection point appeared; with the passage of time this passed into the interior of the k phase. If no extinction occurred, then T_s'' remained positive the whole time, and the temperature profile exhibited no point of inflection. Figure 3 illustrates the time variation in T_s'' for a number of extinction and transient modes.

The condition $T_s'' \leq 0$ is, thus, an essential sign of extinction. However, the satisfaction of this condition does not necessarily mean subsequent extinction of the powder. For an instantaneous fall in pressure, in particular, in the case of a powder model with a variable surface temperature, the temperature gradient φ falls suddenly, whereupon T_s'' passes to $-\infty$ and then remains negative for an appreciable time. Nevertheless, for small depths of pressure drop no extinction takes place.

The physical meaning of the condition under consideration, according to (1.1), lies in the fact that, in the region in which the second derivative of the temperature with respect to the coordinate is negative, there is no heating of the powder particles as they move toward the surface.

4. As a result of our calculations of transient combustion during a pressure drop with various values of p_k and Δt we found the "lines of extinction" for the various versions of the powder model indicated in Table 1, that is, the boundaries expressed in coordinates of (Δt, p_k) above which lay a region in which no extinction ever occurred, and below which lay a region in which a pressure drop always led to extinction. The lines of extinction are illustrated in Fig. 4, in which the points indicate the versions of pressure drop taken from the table – the dark ones in the extinction and the light ones in the transient modes. The existence of lines of extinction for real gunpowder has been confirmed experimentally [1]. As in the experimental determination of such lines, the values of p_k and Δt lying close to the boundaries of the transition are determined by selection.

Let us consider the extinction line I. In coordinates of (Δt, p_k) this consists of segments of straight lines. The extinction line does not pass through the point ($\Delta t = 0$, $p_k = 1$): There is a finite depth of pressure drop at which even after an instantaneous drop the powder continues to burn. For the powder model

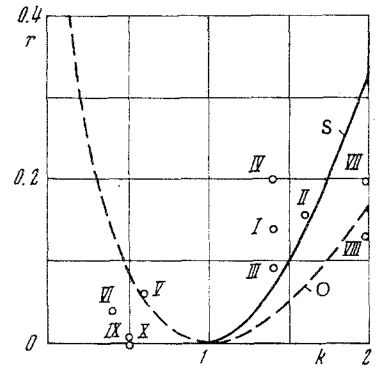

Fig. 5

I the critical depth of the instantaneous drop equaled ~0.15 ($p_k \approx 0.85$), i.e., considerably smaller than would follow from the conclusions of [8], in which extinction was considered as a break in the gas flame as a result of the intensive gasification of the k phase.

For $\Delta t = 2$ the extinction line suffers a break, after which, while remaining linear, it slopes more gently. At the same time, the manner in which the combustion rate varies with time on extinction also changes (curve I-4 in Fig. 2) . First the combustion rate falls in the normal fashion. Subsequently, however, the fall becomes less rapid and ceases almost completely; in individual cases there is even an increase in the combustion rate. The impression is created that the burning process is passing out to a steady operating mode. However, the pressure drop continues, and a new fall in burning rate sets in, leading to extinction. The extinction process in this case develops in two stages and takes longer. Only at the concluding stage is extinction finally determined; then the essential sign of extinction appears: $T_s^* < 0$ (Fig. 3).

The break in the extinction line may be explained by the fact that extinction may occur in either the first or the second period of the fluctuations in the burning rate, and that each form of extinction has its own critical line: the straight line AB in the first case and the straight line BC in the second. Extinction in the second period of the fluctuations occurs when the corresponding critical line is higher, i.e., after the intersection of the lines at the point B. If we continue the straight line AB beyond the intersection (in Fig. 4 this is shown by the broken line), then below this line extinction will occur, as before, by the first mechanism (curve I-5 in Fig. 2).

With increasing Δt the extinction line will undergo further curvature, corresponding to a transition to still more extended extinction processes.

5. Let us consider the influence of the parameters k and m on the extinction process. According to the theory of B. V. Novozhilov [9] the parameters k and m determine the stability of the combustion of gunpowder in the original steady mode of operation. Figure 5 shows the boundaries of the region of stability (line S) in coordinates of (k, $r = k/m$) and the range of existence of characteristic oscillations in the powder (line O). The powder models corresponding to Table 1 are shown as points in Fig. 5.

The extinction lines II and III (Fig. 4) have the same character as the extinction line I, but they lie above it, which indicates extinction for less severe pressure drops. This agrees with the fact that the points II and III in Fig. 5 lie closer to the boundary of stability than the point I. On the other hand, as the powder moves away from the stability boundary the extinction lines lie lower (versions IV, V, VI).

Figure 4 gives the experimental extinction line E for powder of the H type, taken from [1] (case $p_H = 40$ kg/cm^2). Between this line and the results of the calculations, qualitative agreement is clearly seen to exist, especially for version IV. Quantitative agreement is hardly to be expected on using the model relationships (1.4) and (1.5).

We considered the transient combustion of powders in the case in which the original steady mode lay in the region of instability (versions VII and VIII). In the calculations a slight change in pressure was specified (Table 1). The results of the calculations are presented in Fig. 2. In the VII-1 mode we find oscillations of the rate of combustion, with a sharply increasing amplitude, as a result of which extinction takes place even at the second period of oscillations. In the VIII-1 mode, the rate of burning falls monotonically from the very beginning, with greater and greater velocity, until extinction sets in. This difference is explained by the fact that the points VII and VIII in Fig. 5 lie in the regions of the oscillatory and monotonic loss of stability, respectively.

For an unlimited increase in the parameter m, there is a transition to the case of $T_s = \text{const}$ considered by Ya. B. Zel'dovich [3]. In order to realize this case in the calculations we put $m^{-1} = 0$ (version IX). We also considered an intermediate version X in which $m = 100$. The extinction lines in these versions shown in Fig. 4 are quite close to one another.

In the case $T_s = \text{const}$ there is a clearly expressed instant of extinction up to which the rate of burning may be readily calculated. At this instant the solution of the original system of equations vanishes, and the iterative process of the calculation ceases to converge. According to the results of the calculation, the rate of burning falls monotonically, but at the instant of extinction it is nevertheless quite high – extinction occurs abruptly.

In the case m = 100 the rate of burning first diminishes smoothly (curve X-1 in Fig. 2), as in the transient modes. However, at a certain instant of time (in the present case t = 1.94) there is a sharp fall in burning rate to a value of $\sim 10^{-6}$, i.e., extinction sets in. Although the rate of burning changes continuously in time, as in the earlier-considered cases of moderate m values, the character of the extinction is very close to that of a sharp jump. Thus the transition to the case T_s = const occurs continuously, both as regards the form of the extinction line, and as regards the character of the change in burning rate with time.

Extinction was also considered in [5] on the basis of the theory of [2] for a powder model with a constant surface temperature and a constant coefficient of the temperature sensitivity of the rate of steady burning $(\partial \ln u^\circ / \partial T_0)_p$. In contrast to the present investigation, the system of equations describing the transient burning of the powder was solved by the method of integrated relationships, for which purpose the form of the temperature distribution in the k phase was prespecified. A slightly different pressure/time law was also considered. Figure 4 shows the extinction line obtained in [5] for a case coinciding with version IX, converted to coordinates of p_k and Δt (line P). This passes considerably higher than lines IX and X and cuts off at $\Delta t = 1.19$ (according to [5] no extinction occurs for higher values of Δt). This difference is probably associated with the use of the different methods of solving the original equations; the difference in the pressure variation laws is of secondary importance.

6. The assumption as to the existence of limiting points in the φ (p, u) relationship, used in [6, 7] in order to explain extinction, is associated with the means of determining this function from the experimental dependence of the rate of steady combustion on the pressure and initial temperature. The experimental data only enable us to construct a function φ (p, u) in a limited range of variation of the parameters, since outside these limits no states of steady burning can be achieved. This may be explained by the instability of steady-state burning in the region beyond the limiting points, although this does not exclude the possibility of burning in a transient mode [10].

Let us examine the stability of the combustion of gunpowder in the model defined by Eqs. (1.4) and (1.5), which were used in the present investigation. Corresponding to any pair of values φ, u ($u > e^{-m}$) we have a mode of steady burning for a specific pressure and initial temperature. The stability of this mode is determined by the local values of k' and r' [not to be confused with k and r = k/m, the parameters of Eqs. (1.4) and (1.5)]. According to definition [9], the local parameters are related to the derivatives of the functions (1.4) and (1.5)

$$\frac{k' + r' - 1}{k'} = \left(\frac{\partial \ln \varphi}{\partial \ln u}\right)_p, \qquad \frac{r'}{k'} = \frac{u}{p}\left(\frac{\partial T_s}{\partial \ln u}\right)_p$$

Expressing k' and r' in this way and substituting them into the stability criterion [9], we obtain an equation for the stability boundary in coordinates of (u, φ):

$$\left(\frac{\varphi}{u}\right)_y = \frac{2m + k + \sqrt{8mk + k^2}}{2mk}$$

The stability boundary for the case k = 1.4, m = 10 is shown in Fig. 1 (line S). The region of instability of steady-state burning lies to the left of this line. From the experimental determination, the relationship (1.4) could only have been plotted to the right of the stability boundary, and the latter would have entered as a limiting line.

From [9] also follows the equation of the line delimiting the existence of the characteristic oscillations of burning rate in the powder (line O in Fig. 1).

$$\left(\frac{\varphi}{u}\right)_K = \frac{m + k + 2\sqrt{mk}}{mk}$$

The results of these calculations show that the passage of the transient burning process outside the limit of stability does not necessarily mean extinction. This is illustrated by the trajectories of the transient modes I-6 and I-7 in coordinates of (u, φ) presented in Fig. 1. The trajectory I-6 twice intersects the stability boundary, while trajectory I-7 even intersects the boundary limiting the existence of characteristic oscillations (C).

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