CALCULATION OF THE PRESSURE RISE AT A COMBUSTION FRONT

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As a result of the combustion of condensed substances the pressure at their surface may exceed the pressure in the surrounding space, if heat release occurs in the gaseous phase, and also if the flow-off velocity of the gaseous reaction products approximates the velocity of sound.

The corresponding pressure drop is calculated for the case of one-dimensional combustion. Numerical estimates have been made for real condensed substances. The combustion velocity u of condensed systems usually depends on the pressure

$$u = u(p) \tag{1}$$

where p is the pressure in the leading reaction zone, which may be higher than the pressure in the surrounding space p_∞. This, in particular, may be linked with burning of the reaction products in the gaseous phase and also with the fact that the flow-off velocity of the gaseous reaction products does not exceed the velocity of sound.

We shall consider the case when burning of the charge occurs in a sufficiently long casing, and we shall assume that the gas flow and the combustion front are one-dimensional.

The pressure drop associated with burning of the reaction products can be found from the conditions for conservation of mass and momentum flows. Suppose that in the leading reaction zone the temperature is T and the molecular weight of the gas is μ. Suppose that condensed particles are contained in the flow whose velocity is equal to the gas velocity v, and that their weight fraction is m. In addition to T, μ, and m, we are given the flow parameters beyond the combustion zone: T_1, μ_1, and m_1, and also the pressure p_1, which is either equal to or greater than p_∞.

We denote by ρ_*' and ρ_* the particle density and the density of the original condensed system; S is the fraction of the cross-sectional area of the flow occupied by the particles. The initial equations will be:

conservation of mass flow of particles

$$\rho_*' v S = \rho_* u m, \qquad \rho_*' v_1 S_1 = \rho_* u m_1, \tag{2}$$

conservation of mass flow of gas

$$\rho v (1 - S) = \rho_* u (1 - m), \qquad \rho_1 v_1 (1 - S_1) = \rho_* u (1 - m_1), \tag{3}$$

conservation of momentum flow

$$p + \rho_* u v = p_1 + \rho_* u v_1. \tag{4}$$

The normal density of the gas is ρ and ρ_1 is much less than the density of the particles. Taking this into account, we obtain from (2)-(4)

$$(\Delta p)_1 = p - p_1 = \\ = \frac{1}{2}\left[(\rho_* u)^2 \frac{1 - m_1}{\rho_1} - p_1\right] + \left\{\frac{1}{4}\left[(\rho_* u)^2 \frac{1 - m_1}{\rho_1} + p_1\right]^2 - (\rho_* u)^2 \frac{(1 - m) RT}{\mu}\right\}^{1/2}. \tag{5}$$

If $(\Delta p)_1 = p - p_1$ is much less than p_1, we obtain in place of (5)

$$(\Delta p)_1 = (\rho_* u)^2 R \frac{(1 - m_1) T_1/\mu_1 - (1 - m) T/\mu}{p_1 - (1 - m_1)(\rho_* u)^2/\rho_1}. \tag{6}$$

It follows from (5) and (6) that at a very small combustion velocity ($u \to 0$) or for a very slight change in the product $(1 - m)T/\mu$ the pressure drop $(\Delta p)_1$ tends to zero.

We note that in connection with combustion stability the pressure at the surface of the charge p_0 is also of considerable interest. To calculate p_0 it is necessary to sum the pressure drops in all the reaction zones located in the gaseous phase. Thus, for example, for double-flame combustion we get

$$p_0 = p_1 + (\Delta p)_1 + \Delta p, \tag{7}$$

where $(\Delta p)_1$ and p are calculated from (6), and Δp is calculated from the analogous formula

$$\Delta p = (\rho_* u)^2 R \frac{(1 - m) T/\mu - (1 - m_0) T_0/\mu_0}{p - (1 - m)(\rho_* u)^2/\rho}. \tag{8}$$

In (8) the quantities with the subscript 0 refer to the gaseous intermediate products in the gap between the surface of the charge and the leading reaction zone.

We now consider the limitations associated with the fact that the flow-off velocity of the combustion products does not exceed the velocity of sound

$$v \leqslant c = (\gamma RT/\mu)^{1/2}. \tag{9}$$

We substitute v from (2) and (3)

$$v = \rho_* u \left(\frac{1-m}{\rho} + \frac{m}{\rho'_*}\right) \approx \rho_* u \frac{1-m}{p} \frac{RT}{\mu}. \tag{10}$$

It follows from (9) and (10) that the pressure p in the leading reaction zone cannot be lower than a certain minimum value p_{min}

$$p \geqslant p_{min} = (1-m)\,\rho_* u \left(\frac{1}{\gamma} \frac{RT}{\mu}\right)^{1/2}. \tag{11}$$

While the pressure p_∞ is sufficiently large, the gas velocity is usually negligibly small in comparison with the velocity of sound, and the pressure in the leading reaction zone in the absence of burning is equal to the pressure in the space ($p = p_\infty$).

However, if on reducing p_∞ the combustion velocity u diminishes more slowly than linearly, the gas velocity v will increase and for $p_\infty = p_{min}$ it will attain the velocity of sound. Beginning from this instant the pressure p in the leading reaction zone will be constant and equal to p_{min}, independent of any further reduction in p_∞. Correspondingly, the combustion velocity must also remain constant and equal to $u_{min} = u(p_{min})$.

In the presence of burning v, c, T, p, etc., should be replaced in formulas (9)-(11) by v_1, c_1, T_1, p_1, etc. In other words, in this case the pressure p_1 behind the burning zone cannot be less than $(p_1)_{min}$

$$p_1 \geqslant (p_1)_{min} = (1-m_1)\,\rho_* u \left(\frac{1}{\gamma_1} \frac{RT_1}{\mu_1}\right)^{1/2}. \tag{12}$$

In this case the pressure in the leading reaction zone will be equal to $(p_1)_{min} + (\Delta p)_1$, where $(\Delta p)_1$ is calculated from (5) and (6).

We shall now make certain numerical estimates. For pressures which are not too low, the pressure drop, because of the presence of burning, can play a significant role only in fast-burning systems. Thus, according to the data of [1, 2], the combustion of mercury fulminate ($\rho_* = 3.8$ g/cm^3) proceeds in two stages. In the first stage only 10-20% of the original substance is decomposed and 80-90% is dispersed and burns at a considerable distance from the surface of the charge.

The combustion velocity is determined by the first low-temperature (~ 500°C) stage. For the second stage, a provisional thermodynamical calculation (without taking into account dissociation) starting from the reaction equation

$$Hg(ONC)_2 \rightarrow Hg + 2CO + N_2$$

gives a value $T_1/\mu_1 \approx 52$. For $p_\infty = 1$ atm the experimental value $u \simeq 1.5$ cm/sec. The corresponding pressure drop, associated with burning, amounts [according to formula (5)] to about 170 mm Hg. For $p_\infty <$ 40-50 mm Hg the second flame dies out. The value of p_{min} at which the velocity of the products from this single-stage combustion should approximate the velocity of sound, according to formula (9), is 4-8 mm Hg (without taking into account the effect of solid particles on the velocity of sound). In other words, as a result of the combustion of mercury fulminate in a casing in vacuo, the pressure at its surface cannot fall below 4-8 mm.

A significantly higher pressure p_{min} should occur for lead styphnate. According to data from [3], the combustion velocity of lead styphnate ($\rho_* = 3.8$ g/cm^3) is very weakly dependent on p_∞, increasing from 25-26 cm/sec at p_∞ = = 15 mm Hg to 33-35 cm/sec at $p_\infty = 400$ atm. The value of p_{min}, calculated from formula (11), is about 4 atm for lead styphnate.* The lack of dependence of u on p_∞ for lead styphnate at high values of p_∞ must be connected with the

*In the computations we used the data of the approximate thermodynamic calculation (without taking into account dissociation) for the reaction

$$C_6H_3N_3O_9Pb \rightarrow 1.5\,H_2O + 5.5\,CO + 0.5\,CO_2 + 1.5\,N_2 + PbO$$

For $p = p_{min}$ (p_{min} is found by the method of successive approximations) we obtained $T \approx 1530$°K, $\mu \approx 31.8$, $m \approx$ ≈ 0.37 (part of the PbO is found in the combustion products in the form of particles). The effect of the particles on the velocity of sound was not taken into account.

combustion mechanism, but at values of p_∞ below a few atmospheres it may be connected with the constancy of the pressure at the combustion surface. It should be noted that if even insignificant burning of the reaction products occurs for lead styphnate, then this may increase significantly (by several atmospheres) the pressure at its surface.

For secondary explosives and powders the combustion velocity is considerably lower (according to the data of [4], at 1 abs atm it lies within the limits 0.01 to 0.3 cm/sec). Consequently, the pressure drop associated with burning may play a significant role only as a result of combustion in vacuo. The value of p_{min} is also small (for the flameless combustion of pyroxylin powder studied in [5], the calculations give $p_{min} \approx 1$ mm Hg).

Above we considered one-dimensional combustion. If the charge burns without a casing, the combustion front ceases to be one-dimensional, but the flow, obviously, must include a rarefaction wave in order to satisfy the boundary conditions at the combustion front. The shape of the front as a result of such combustion has not been specially investigated therefore the calculations are also indeterminate.

It is obvious only that the increase in pressure in the example of a charge without casing is lower than in the example of a cased charge, and it diminishes with increase in the distance between the combustion zone and the surface of the charge. Conversely, if the combustion zone is situated sufficiently close to the surface of the charge, combustion differs little from the one-dimensional case. This is confirmed by experimental observations, according to which the surface of burning charges (without casing) may remain plane, providing the combustion takes place in an inert atmosphere and the combustion products do not flow around the lateral surface of the charge.

As an example we may consider the configuration when the leading zone and the surface of the charge are plane, but the combustion zone forms a conical front with an angle α at the vertex. In this case the pressure drop associated with burning of the gaseous reaction products ($m = m_1 = 0$) can be found from (5) and (6), where $(\rho_* u \sin \alpha/2)^2$ must be substituted in place of $(\rho_* u)^2$. Correspondingly, for $\alpha = 90°$ the pressure drop is half that for a one-dimensional front; for $\alpha = 60°$ it is four times less, etc.

In conclusion we may make the following comments.

The increase of pressure at the surface of a burning charge is calculated in [4] from the condition

$$Ft = p_* uv \approx \frac{(\rho_* u)^2}{\rho} \qquad (F = \Delta p \cdot 1\text{cm}^2). \tag{13}$$

Although this method enables the order of magnitude of Δp to be estimated, it is not correct. Actually, F in (13) has the significance of a reactive force acting on the surface of the charge. The existence of F does not at all require the presence of a pressure increase at the surface of the charge (and does not permit Δp to be calculated). This is particularly obvious in the case when no gaseous products at all are formed during combustion, but part of the solid products are dispersed because of the occurrence of thermal stresses. Then F fully preserves its significance and can be calculated from an expression similar to (13), while Δp (and if combustion takes place in vacuo, p also) identically vanish (in the same way Δp will be equal to zero, if the reaction takes place entirely in the condensed phase with the formation of gaseous end products, without burning in the gaseous phase, and on condition that the gas velocity is less than the velocity of sound).

Accordingly, it is not possible to acknowledge the correctness of the experimental method for determining Δp, in which the force F acting from the direction of the charge is measured by means of spring-loaded weights, etc. and it is assumed that $\Delta p = F/S$, where S is the cross-sectional area of the charge.

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