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Fig. 1

Figure 1: Fig. 1

Abstract

Full Text

PHYSICAL CHEMISTRY

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ON THE STABILITY OF DETONATION WAVES IN GAS MIXTURES

(Presented by Academician Ya. B. Zel'dovich on 18 VIII 1960)

The study of the stability of a detonation wave (d.w.) is of interest for explaining spin detonation. As shown in ¹, in the kink of a d.w. there is an overcompression, in the region of which the combustion of the mixture is accelerated. On the basis of these ideas, in ² qualitative criteria of instability were obtained for a d.w.; this instability also occurs far from the detonation limits. At the same time, as experiments ³ have shown, a multiheaded spin arises. In the present work the stability of a d.w. with respect to small perturbations is considered.

Let the d.w. propagate from right to left, and let the frame of reference be chosen so that the wave front is at rest and coincides with the plane YOZ of a Cartesian coordinate system. The axis OX coincides with the direction of gas motion (see Fig. 1). We shall assume, as in ², that in the zone of the chemical peak (region 1) all quantities are constant, and that at a distance $L = v_1\tau$ from the d.w. front the reaction occurs instantaneously, so that the final state 2 is reached by a jump. In region 2 the quantities p_2, ρ_2, v_2 are also regarded as constant, since with the passage of time the gradients of all quantities become arbitrarily small. For simplicity we shall assume that the gas is ideal and that its heat capacity is constant. The isentropic exponent γ before the reaction (in regions 0 and 1) and after the reaction (region 2) is equal, respectively, to γ_1 and γ_2 . Without loss of generality, one may assume that the perturbations depend only on x, y, t , and that the velocity component along the OZ axis is zero.

Fig. 1

The solution of the linearized hydrodynamic equations in region 1 will be the sum of terms of the form

$A_s \exp[i(k_s x + k_0 y - \omega t)]$ ($s = 1, 2, 3$), where k_0 is a given wave number; ω is the eigenfrequency sought; A_s are constants; $k_1 = \omega/v_1$; k_2 and k_3 are found from the equation

$$(v_1 k - \omega)^2 - c_1^2(k_0^2 + k^2) = 0.$$

Similarly, in region 2 the solution will contain terms of the form $B_s = \exp[i(q_s x + k_0 y - \omega t)]$ ($s = 1, 2, 3$), where B_s are constants; $q_1 = \omega/v_2$; q_2 and q_3 are found from the equation

$$(v_2 q - \omega)^2 - c_2^2(k_0^2 + q^2) = 0.$$

In an overcompressed d.w. ($v_2 < c_2$) in region 2, perturbations may propagate both with the gas flow ($q = q_2$) and against the flow ($q = q_3$). The problem is to find such values of ω for which a nontrivial solution exists under the condition that the amplitude of the wave coming from infinity to the front is zero. In studying the stability of a d.w. in the Chapman-Jouguet regime, the calculations in essen—

do not change. Such a formulation corresponds to the problem of the passage of a sound wave incident against the detonation wave, under the condition that the amplitude of the incident sound wave is set equal to zero.

Let $\varepsilon_1(y, t) = \Delta_1 \exp[i(k_0 y - \omega t)]$ be the displacement of the shock-wave front ($x = 0$); $\varepsilon_2(y, t) = \Delta_2 \exp[i(k_0 y - \omega t)]$ the displacement of the reaction front ($x = L$); Δ_1 and Δ_2 are constants. The boundary conditions for the perturbations at $x = 0$ and $x = L$ are obtained (similarly to how this was done in (4)) by varying the conditions of continuity of the fluxes of mass, momentum, energy, and of the tangential component of velocity. We shall characterize the reaction kinetics by a delay time τ , which depends on the effective values of the pressure and temperature in the chemical spike. Let the reaction process in a given gas particle be described by the equation:

$$d\psi/dt = f(p; T), \quad (1)$$

where ψ is the concentration of one of the components of the mixture. If in some gas particle the reaction began at time t , then it will end at time $t + \tau$. Integrating (1), we obtain:

$$\psi_2 - \psi_1 = \int_t^{t+\tau} f(p_1; T) dt', \quad (2)$$

where ψ_1 and ψ_2 are the concentrations of the given component in the initial mixture and in the reaction products, respectively. We assume that, also in the presence of perturbations, the reaction proceeds to completion; then the variation of ψ_1 and ψ_2 gives zero. Our approximation consists in replacing, in the unperturbed motion, the true pressure and temperature profiles by constant values: $p = p_1$, $T = T_1$. Instead of (2) we shall then have $\psi_2 - \psi_1 = f(p; T_1)\tau$. In the presence of perturbations condition (2) takes the form

$$\psi_2 - \psi_1 = \int_t^{t+\tau+\tau'} f(p_1 + p'_1; T_1 + T'_1) dt'. \quad (3)$$

Here τ' is a small change in the delay time caused by perturbations of pressure and temperature (p'_1 and T'_1) in region 1. Introduce the notation: $M = \partial \ln f / \partial \ln p$; $N = \partial \ln f / \partial \ln T$ (the derivatives are taken at $p = p_1$, $T = T_1$). Restricting ourselves to terms of first order, from (2) and (3) we find

$$\tau' = - \int_t^{t+\tau} \left(M \frac{p'_1}{p_1} + N \frac{T'_1}{T_1} \right) dt'. \quad (4)$$

The integration with respect to dt' is performed along the trajectory of the given particle. In the unperturbed motion the trajectory was the line $x = v_1(t' - t)$, where t is the instant at which the particle passes through the shock-wave front. The presence of perturbations bends the particle trajectory by a quantity of first order. In calculating τ' , this correction may be neglected. During the time from t to $t + \tau + \tau'$, along the OX axis the particle will travel the distance

$$l = \int_t^{t+\tau+\tau'} (v_1 + v'_{1x}) dt' \simeq L + v_1\tau' + \int_t^{t+\tau} v'_{1x} dt', \quad (5)$$

where v'_{1x} is the perturbation of the x -component of velocity. If the reaction began in the particle at time t at the point $\varepsilon_1(t)$, then the reaction will end at time $t + \tau + \tau'$ at the point $x = L + \varepsilon_2(t + \tau + \tau') \simeq L + \varepsilon_2(t + \tau)$, and during this time the particle will travel from its initial position $\varepsilon_1(t)$ the distance l , i.e. $\varepsilon_1(t) + l = L + \varepsilon_2(t + \tau)$. Substituting (4) and (5) here, we write the desired condition in the form:

$$v \int_t^{t+\tau} \left(M \frac{p'_1}{p_1} + N \frac{T'_1}{T_1} - \frac{v'_{1x}}{v_1} \right) dt' - \varepsilon_1(t) + \varepsilon_2(t + \tau) = 0.$$

The integral is taken along the line $x = v_1(t' - t)$. The displacement of particles along the OY axis in the linear approximation may be neglected.

Substitution of the solutions into the boundary conditions leads to a system of 9 linear homogeneous equations. The condition that the determinant of this system be equal to zero can be written in the form

$$G_2 D_3 - G_3 D_2 = 0, \quad (6)$$

where the following notation has been introduced:

$$\begin{aligned}
 G_s &= \frac{\omega}{a_s} \left[1 + \left(\frac{\omega}{k_0 v_1} \right)^2 \right] + \frac{1-\delta}{2} \left[\frac{v_0}{v_1} + \left(\frac{\omega}{k_0 v_1} \right)^2 \right], \\
 D_s &= \frac{E}{a_s} - \frac{v_0 - v_1}{1 + (\omega/k_0 v_1)^2} \left[1 + \frac{v_1}{v_0} \left(\frac{\omega}{k_0 v_1} \right)^2 \right] E_s R^s, \\
 E_s &= \left(\mu - \frac{v_1^2}{c_1^2} + 1 + \frac{\omega}{a_s} \right) \frac{F_1}{v_1 a_s} - \frac{F_s}{c_2^2}, \\
 F_s &= \frac{1-\alpha}{2\alpha} \left(h_2 - \frac{v_0}{v_2} \right) \left\{ \frac{k_0}{a_s} \left[1 + \left(\frac{\omega}{k_0 v_1} \right)^2 \right] \right. \\
 &\quad \left. - \frac{\omega}{k_0 v_1} \left(\frac{1}{v_1} - \frac{1}{v_2} \right) \left(\frac{2\omega v_2}{a_s v_1} + 1 - \frac{v_1^2}{c_1^2} \right) \right\} \\
 &\quad - \frac{k_0}{2(v_2 q_2 - \omega)} \left[1 + \left(\frac{\omega}{k_0 v_2} \right)^2 \right] \left\{ \frac{c_2^2}{\gamma_2 v_1^2} \left(h_2 + \frac{p_1}{p_2} \right) \left[\left(1 - \frac{v_1}{v_2} \right) \frac{2\omega}{a_s} \right. \right. \\
 &\quad \left. \left. + \left(2 - \frac{v_1}{v_2} \right) \left(1 - \frac{v_1^2}{c_1^2} \right) \right] + \left(\frac{v_2}{v_1} - 1 \right) \left(1 - \frac{v_1^2}{c_1^2} \right) \right\},
 \end{aligned} \tag{7}$$

$$R_s = e^{i a_s \tau} - 1, \quad a_s = v_1 k_s - \omega, \quad s = 2, 3;$$

$$\begin{aligned}
 E &= i\omega\tau \left(\frac{1}{v_1} - \frac{1}{v_0} \right) \left[\frac{v_0 - v_1}{1 + (\omega/k_0 v_1)^2} + \frac{2v_1 N}{1-\delta} \left(\frac{v_1^2}{c_1^2} - \delta \right) \right] F_1 + F_0, \\
 F_0 &= \frac{k_0}{\gamma_2} \left(\frac{1}{v_2} - \frac{1}{v_0} \right) \left(h_2 + \frac{p_0}{p_2} \right) \left\{ \frac{\omega}{v_2 q_2 - \omega} \left[1 + \left(\frac{\omega}{k_0 v_2} \right)^2 \right] + \frac{1-\alpha}{2} \left[\frac{v_0}{v_2} + \left(\frac{\omega}{k_0 v_2} \right)^2 \right] \right\}, \\
 F_1 &= \frac{k_0}{\gamma_2} \left(\frac{1}{v_1} - \frac{1}{v_2} \right) \left\{ \frac{\omega}{v_2 q_2 - \omega} \left[1 + \left(\frac{\omega}{k_0 v_2} \right)^2 \right] \left(h_2 + \frac{p_1}{p_2} \right) \right. \\
 &\quad \left. + \frac{h_2 + 1}{2} \left(1 - \frac{v_2^2}{c_2^2} \right) \left[\frac{v_1}{v_2} + \left(\frac{\omega}{k_0 v_2} \right)^2 \right] \right\},
 \end{aligned} \tag{8}$$

$$h_1 = \frac{\gamma_1 + 1}{\gamma_1 - 1}, \quad h_2 = \frac{\gamma_2 + 1}{\gamma_2 - 1}, \quad \mu = \gamma_1 M + (\gamma_1 - 1)N,$$

$$\delta = -j^2 \left(\frac{\partial V_1}{\partial p_1} \right)_H = \frac{c_0^2}{v_0^2}, \quad \alpha = -j^2 \left(\frac{\partial V_2}{\partial p_2} \right)_H = j^2 \frac{h_2 V_2 - V_0}{h_2 p_2 + p_0},$$

$$V_0 = 1/\rho_0, \quad V_1 = 1/\rho_1, \quad V_2 = 1/\rho_2, \quad j = \rho_0 v_0.$$

In the case when the reaction zone is small in comparison with the wavelength of the perturbation ($k_0 L \ll 1$), putting $\tau = 0$, instead of (6) we obtain

$$\frac{\omega}{v_2 q_2 - \omega} \left[1 + \left(\frac{\omega}{k_0 v_2} \right)^2 \right] + \frac{1 - \alpha}{2} \left[\frac{v_0}{v_2} + \left(\frac{\omega}{k_0 v_2} \right)^2 \right] = 0. \quad (9)$$

Considering the case of a very broad reaction zone ($k_0 L \gg 1$), let us note that, in seeking conditions leading to instability, we assume that $\text{Im } \omega > 0$. In this case the functions $\exp[i(k_2 x + k_0 y - \omega t)]$ and $\exp[i(k_3 x + k_0 y - \omega t)]$, respectively, decrease and increase exponentially with increasing coordinate x . Therefore, for $k_0 L \gg 1$ we have $|R_3| \gg |R_2|$ and $|D_3| \gg |D_2|$. Instead of (6) we obtain $G_2 = 0$, i.e.

$$\frac{\omega}{v_1 k_2 - \omega} \left[1 + \left(\frac{\omega}{k_0 v_1} \right)^2 \right] + \frac{1 - \delta}{2} \left[\frac{v_0}{v_1} + \left(\frac{\omega}{k_0 v_1} \right)^2 \right] = 0. \quad (10)$$

In their form, (9) and (10) coincide with the characteristic equation obtained by S. P. D' yakov⁽⁴⁾. Using his results, we find that in the two limiting cases considered the detonation wave is stable. Instability, however, can manifest itself only for $k_0 L \sim 1$, which is, of course, obvious.

Let $\omega = 0$ for $k_0 = \varkappa$. It can be shown that \varkappa will be real under the condition

$$\mu \left(\frac{v_2}{v_1} - 1 \right) \frac{v_1^2}{c_1^2} > 2 - \frac{v_2}{v_1} + \left[2 \frac{v_2}{v_1} - 1 + (\gamma_2 - 1) \left(\frac{v_2}{v_1} - 1 \right) \frac{v_2^2}{c_2^2} \right] \sqrt{\frac{1 - v_1^2/c_1^2}{1 - v_2^2/c_2^2}}. \quad (11)$$

If now in equation (6) one expands in powers of ω and $k_0 - \varkappa$, then in a neighborhood of the point $k_0 = \varkappa$ the quantity $\Omega = -i\omega$ will be positive. Thus, condition (11) is sufficient for the overdriven detonation wave to be unstable.

Let us consider a detonation wave in the Chapman–Jouguet regime: $v_2 = c_2$. For simplicity we shall assume that $p_0 = 0$; $\gamma_1 = \gamma_2 = (h + 1)/(h - 1)$. Then equation (6) takes the form

$$\frac{1}{2} w(u_2 - u_3) B + \Phi_2 \Psi_2 R_2 - \Phi_3 \Psi_3 R_3 = 0, \quad (12)$$

where

$$B = h - \frac{(h - 1)(h + 2)}{h + 1} \left(\frac{h^2 - 1}{1 - w^2} + 2N \right) w\xi,$$

$$\Phi_s = w(u_s - w) - \frac{h+1}{2h}(h - w^2),$$

$$\Psi_s = (h-1)(h+2) \left(\frac{\mu}{h+1} + 2 + \frac{w}{u_s - w} \right) \frac{w}{u_s - w} + h(h+1), \quad (13)$$

$$R_s = e^{-\xi(u_s - w)} - 1, \quad s = 2, 3, \quad w = \Omega/k_0 v_1, \quad \xi = k_0 v_1 \tau,$$

$$u_{2,3} = [-w \pm \sqrt{(h+1)(h+w^2)}] / h.$$

Denote by $F(w)$ the left-hand side of equation (12). Then $F(0) > 0$, and $F(1)$ is bounded. As $w \rightarrow +\infty$, $R_3 \gg R_2 \gg 1$; therefore, if

$$\mu > (h+3)(h+1 + \sqrt{h+1}) / (h-1)(h+2), \quad (14)$$

then $F(+\infty) < 0$, i.e., equation (12) will have a root $w > 0$. Thus, condition (14) is sufficient for instability of a detonation wave in the Chapman–Jouguet regime. We note that in the example given in ⁽²⁾, condition (14) leads to the inequality $4.80 > 2.17$. Thus, in the indicated case the detonation wave is unstable, which confirms the conclusions of K. I. Shchelkin.

For a more detailed investigation of the characteristic equation (6), numerical methods are necessary. This task is facilitated by the fact that equation (6) can be solved with respect to the parameter N (or M). Then, varying the complex number ω along a certain contour, one should seek such a value of it for which $N(\omega)$ becomes real (positive).

In conclusion I express my gratitude to Academician Ya. B. Zel' dovich for proposing the topic and for his constant interest in the work.

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CITED LITERATURE

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

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