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**Abstract****Full Text**

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**PHYSICAL CHEMISTRY**

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**A CRITERION FOR THE INSTABILITY OF  
CHAPMAN–JOUQUET DETONATION IN A  
GAS**

*(Presented by Academician E. K. Zavoisky, 8 I 1965)*

The stability of a plane stationary detonation propagating through a gaseous mixture has been studied theoretically in works <sup>(1–4)</sup>. K. I. Shchelkin <sup>(1)</sup>, from qualitative considerations, obtained a criterion for the instability of a detonation wave that agrees with experiment. In work <sup>(4)</sup> the resulting eigenvalue problem was solved numerically. The mathematical analysis of the stability problem carried out in <sup>(2,3)</sup> also did not lead to a general criterion. In the present work, an analytic method establishes, in general form, a criterion for the instability of Chapman–Jouquet detonation.

We use the model of K. I. Shchelkin <sup>(1)</sup>, which represents the detonation wave in an ideal gas as a stationary complex that includes a shock wave and, following it at a certain distance  $L$ , the front of an instantaneous chemical reaction with characteristic delay time  $\tau$ . The three resulting flow regions with constant parameters  $p, \rho, v, T, S, a, c_p, \chi$  (respectively, pressure, density, velocity, temperature, entropy, speed of sound, heat capacity, and isentropic exponent) will be denoted by the indices 0, 1, 2 (respectively, the initial mixture, the shock-compressed gas, and the detonation products). The axis  $y$  corresponds to the stationary state of the shock front; the ignition front occupies the position  $x = L$ . The pressure, velocity, and entropy are chosen as the basic variables, and it is assumed that in the presence of disturbances the chemical reaction proceeds to completion. Then linearization of the laws of continuity of the fluxes of mass, momentum, and energy at an arbitrary discontinuity <sup>(5)</sup> (generally speaking, taking chemical transformations into account) leads to the following equations for the disturbances:

$$\begin{aligned}
 v'_{jx} - (1 - \alpha_j) \frac{\partial \varepsilon_j}{\partial t} + \frac{p'_j}{\rho_1 v_1} M_j^2 - \frac{v_j}{c_{pj}} S'_j &= \\
 &= \alpha_j \left( v'_{j-1,x} + \frac{p'_{j-1}}{\rho_1 v_1} M_{j-1}^2 - \frac{v_{j-1}}{c_{pj-1}} S'_{j-1} \right), \tag{1}
 \end{aligned}$$

$$\frac{p'_j}{\rho_1 v_1} (1 + M_j^2) + 2v'_{jx} - \frac{v_j}{c_{pj}} S'_j = \frac{p'_{j-1}}{\rho_1 v_1} (1 + M_{j-1}^2) + 2v'_{j-1,x} - \frac{v_{j-1}}{c_{pj-1}} S'_{j-1},$$

$$v'_{jy} + (\alpha_j - 1) v_{j-1} \frac{\partial \varepsilon_j}{\partial y} = v'_{j-1,y},$$

$$\begin{aligned}
 v'_{jx} - \left( 1 - \frac{1}{\alpha_j} \right) \frac{\partial \varepsilon_j}{\partial t} + \frac{p'_j}{\rho_1 v_1} + \frac{v_j}{c_{pj}} S'_j \frac{1}{(\chi_j - 1) M_j^2} &= \\
 &= \frac{1}{\alpha_j} \left[ v'_{j-1,x} + \frac{p'_{j-1}}{\rho_1 v_1} + \frac{v_{j-1}}{c_{pj-1}} S'_{j-1} \frac{1}{(\chi_{j-1} - 1) M_{j-1}^2} \right],
 \end{aligned}$$

where  $M_j = v_j/a_j$  is the Mach number;  $\alpha_j = v_j/v_{j-1} = \rho_{j-1}/\rho_j$ , and  $\varepsilon_j$  is the displacement of the discontinuity in the disturbed state. For  $x = 0$  and  $j = 1$ , the latter give boundary conditions for the shock front, if one takes into account  $p'_0 = v'_{0x} = v'_{0y} =$

$= S'_0 = 0$ . For  $x = L = v_1 \tau$  and  $j = 2$ , conditions (1) become the boundary conditions for the flame front. The kinetics of the chemical reaction imposes on the perturbations the requirement (2)

$$\int_t^{t+\tau} \left[ m M_1^2 \frac{p'_1}{\rho_1 v_1} + N \frac{v_1}{c_{p1}} S'_1 - v_1 x' \right]_{x=v_1(t'-t)} dt' - \varepsilon_1(t) + \varepsilon_2(t + \tau) = 0, \tag{2}$$

$$m = \varkappa_1 Q + (\varkappa_1 - 1) N, \quad Q = \left. \frac{\partial \ln f}{\partial \ln p} \right|_{T=T_1}^{p=p_1}, \quad N = \left. \frac{\partial \ln f}{\partial \ln T} \right|_{T=T_1}^{p=p_1}.$$

$f(p, T)$  is the rate of the chemical reaction. The boundary condition as  $x \rightarrow +\infty$  consists in the boundedness of the perturbations. The solution of the linearized gas-dynamic equations in regions 1, 2 ( $j = 1, 2$ ) is represented in the form

$$v'_{jx} = (2 - j) A_j \Phi_{j-1} + A_{j+1} \Phi_j + A_{j+3} \Psi_j,$$

$$\begin{aligned}
 v'_{jy} &= (2-j) \frac{i}{\gamma_{j-1}} A_j \Phi_{j-1} + \frac{i}{\gamma_j} A_{j+1} \Phi_j - \frac{\omega}{kv_j} A_{j+3} \Psi_j, \\
 \frac{p'_j}{\rho_1 v_1} &= \left( \frac{i\omega}{kv_j \gamma_{j-1}} - 1 \right) (2-j) A_j \Phi_{j-1} + \left( \frac{i\omega}{kv_j \gamma_j} - 1 \right) A_{j+1} \Phi_j, \quad (3) \\
 S'_j &= \frac{c_{pj}}{v_j} A_{j+5} \Psi_j, \quad \Phi_j = \Psi_0 \exp(k\gamma_j x), \quad \Psi_j = \Psi_0 \exp\left(\frac{i\omega}{v_j} x\right), \\
 \varepsilon_j &= \frac{1}{kv_1} A_{j+7} \Psi_0, \quad \Psi_0 = \exp(iky - i\omega t);
 \end{aligned}$$

where

$$\begin{aligned}
 (1 - M_1^2) \gamma_{0,1} &= z M_1^2 \pm \sqrt{1 - M_1^2 + z^2 M_1^2}, \\
 z &= -\frac{i\omega}{kv_1}, \quad (4) \\
 (1 - M_2^2) \gamma_2 &= \frac{z}{\alpha_2} M_2^2 \pm \sqrt{1 - M_2^2 + \frac{z^2}{\alpha_2^2} M_2^2},
 \end{aligned}$$

$\lambda = 2\pi/k$  is the wavelength of the perturbation at the discontinuities. The choice of the branch  $\gamma_2$  is made according to the condition  $\text{Re}(\gamma_2) \leq 0$  as  $x \rightarrow +\infty$ .

As a result of substituting the solution (3) into conditions (1), (2), the following characteristic equation for the eigenfrequency  $\omega$  is obtained:

$$\begin{aligned}
 z \left( \frac{z^2}{\alpha_2^2} - 1 \right) (\varphi_1 \varphi_3 - \varphi_2 \varphi_4) &= 0, \\
 \varphi_1 &= (1 - M_1^2) \left( \frac{1}{\gamma_0} - \frac{1}{\gamma_1} \right), \quad \varphi_2 = \frac{1}{\gamma_0} B_1 + E_0 C_0, \\
 \varphi_3 &= B_1 \delta_4 + D_0 [\delta_4 z + \xi \beta (\alpha_2 - 1) B_0 - (z^2 - 1) E_1] + \gamma_0 E_0 (\delta_2 C_0 - D_0 F_0) \\
 &\quad - D_1 \left\{ \delta_4 [1 - z^2 + (B_0 - 3)(\alpha_2 - 1)] - \frac{\alpha_1 \alpha_2 - 1}{\alpha_1 - 1} (z^2 - 1) \right. \\
 &\quad \left. + \frac{z}{\alpha_2} (\alpha_2 - 1) [\delta_4 z + \xi \beta (\alpha_2 - 1) B_0 - (z^2 - 1) E_1] \right. \\
 &\quad \left. + E_0 \gamma_0 (\alpha_2 - 1) \left( \delta_2 G_0 - \frac{z}{\alpha_2} F_0 \right) \right\}, \quad (5)
 \end{aligned}$$

$$\varphi_4 = c_1 \delta_3 - D_0 F_1 + \frac{\gamma_0}{\gamma_1} (D_0 F_0 - \delta_2 C_0) - D_1 \left\{ \delta_3 (\alpha_2 - 1) G_1 + (\alpha_2 - 1) \left[ -\frac{z}{\alpha_2} F_1 + \frac{\gamma_0}{\gamma_1} \left( \frac{z}{\alpha_2} F_0 - \delta_2 G_0 \right) \right] \right\},$$

$$B_r = 2^r - (\nu_1 - 1) M_1^2 N^{1-r} (z^2 - 1), \quad C_r = 1 - M_1^2 - (1 + M_1^2) \frac{z}{\gamma_r},$$

$$D_0 = (1 - M_2^2) \gamma_2 - (1 + M_2^2) \frac{z}{\alpha_2}, \quad E_0 = \frac{\alpha_1 z^2 - 1}{(\alpha_1 - 1) z},$$

$$E_1 = \frac{\alpha_1 [1 + \beta (\alpha_2 - 1)] - 1}{(\alpha_1 - 1)^2 z}.$$

$$D_1 = 2 + (\nu_2 - 1) M_2^2 - \frac{(1 - M_2^2) z / \alpha_2}{z / \alpha_2 \mp \sqrt{1 - M_2^2 + (z^2 / \alpha_2^2) M_2^2}}, \quad \beta = \exp(-\xi z),$$

$$F_r = \frac{\delta_{r+2}}{\gamma_r} - \delta_r \beta (\alpha_2 - 1) \left[ 1 + m M_1^2 \left( 1 + \frac{z}{\gamma_r} \right) \right],$$

$$G_r = M_1^2 \frac{z}{\gamma_r} - 1 + M_1^2, \quad \delta_l = \frac{\exp \xi (z + \gamma_l) - 1}{z + \gamma_l} \quad (l = 0, 1),$$

$$\delta_{l+2} = \exp \xi \gamma_l - 1, \quad \delta_4 = \beta - 1, \quad \xi = kL = 2\pi L / \lambda,$$

where the signs in  $D_1$  and  $\gamma_2$  are opposite. The root (5)  $z = \alpha_2$  is rejected on physical grounds. In the limiting case of vanishing thickness of the detonation zone ( $\xi = 0$ ), the complex under study turns into the classical scheme of a jump with an energy influx. Equation (5) is simplified and, with the aid of the change of variable ( $j = 2$ ),

$$z = \frac{\eta_j}{M_j} \operatorname{sh} u, \quad \gamma = \frac{1}{\eta_j} (M_j \operatorname{sh} u \pm \operatorname{ch} u), \quad \eta_j = \sqrt{1 - M_j^2} \quad (j = 1, 2) \quad (6)$$

takes the form

$$A \operatorname{cth}^2 u + 2B \operatorname{cth} u + C = 0. \quad (7)$$

Analysis of the roots of the resulting quadratic equation shows that only  $\operatorname{Re} z \leq 0$  can occur, i.e., neutral oscillations. To clarify the influence of the finiteness of the detonation zone on stability, we confine ourselves to the most interesting

case of Chapman–Jouguet detonation ( $M_2 = 1$ , in  $\gamma_2$  only the minus sign). Seeking the solution of (5) in the form of a power expansion  $z = z_0 + z_1\xi + \dots$ , we find

$$z_0 = z_2 = 0, \quad z_1 = \alpha_2 \frac{\alpha_1 - 1}{\alpha_1 \alpha_2 - 1} \frac{1 + (\nu_2 + 1)(\alpha_2 - 1)}{\nu_2 - 1 - (\nu_2 + 1)\alpha_1 \alpha_2} \quad (\alpha_1 < 1, \alpha_2 > 1).$$

According to the classical theory of detonation, the latter is always negative. Thus, to an accuracy up to  $\xi^3$ , instability will be absent. In the other limiting case, where  $\lambda$  is large relative to the width of the detonation zone ( $\xi \gg 1$ ), it is already possible to obtain the instability condition  $\text{Re } z > 0$  as a function of the chemical kinetics, in contrast to the erroneous assertion of work (2) concerning absolute stability for the given assumption. From (4) it follows at once that one of  $\gamma_{0,1}$  (let it be  $\gamma_0$ ) has the largest real part, which is positive. Therefore, in the case under consideration, all terms of (5) will be exponentially small in comparison with those containing the factors  $\delta_2 = \delta_0 \beta(z + \gamma_0)$ , which have order  $\exp \xi \gamma_0$ . Then, retaining the principal terms in (5), we arrive, for the Chapman–Jouguet regime, at the following:

$$\begin{aligned} & \{B_0 + E_0[(1 - M_1^2)\gamma_1 - (1 + M_1^2)z]\} \times \\ & \times \{z^2(q_1 + \mu q_2) + \gamma_0^2(q_1 + \alpha_2 q_2) + z\gamma_0[2q_1 + (\mu + 1)q_2]\} = 0, \quad (8) \\ & q_1 = M_1^2[\nu_2 - \alpha_2(\nu_2 + 1)] - 1, \quad \alpha_2 q_2 = 2 + (\nu_2 + 1)(\alpha_2 - 1), \end{aligned}$$

$$\mu = 1 - m M_1^2 (\alpha_2 - 1).$$

The error of the approximation used will be estimated below. Applying the substitution (6) (for  $j = 1$ ) reduces both square brackets of (8) to equations of the form (7). The investigation of the roots of these equations is carried out analogously. The first bracket coincides exactly with the characteristic equation for the shock wave separating regions 0 and 1, and gives imaginary values of the eigenvalue  $z$ , ensuring neutral oscillations. For the second bracket of (8), complex values of  $z$  always ensure stability of the process. Analysis of real  $z$  leads, in the final analysis, to the follow-

the instability criterion for Chapman–Jouguet detonation with respect to small perturbations:

$$m \frac{q_2 M_1^2 (\alpha_2 - 1)}{(M_1 + 1)(q_2 - 1)} > 1. \quad (9)$$

The latter was obtained by retaining in (5) terms of order  $\exp \xi \gamma_0$ . The real character of  $z$  and  $\gamma_0 > 0$  require the plus sign in (7), and hence  $\gamma_0 > 1/\eta_1$ . The large value of the detonation velocity gives (for a diatomic gas)  $1/\eta_1 = \sqrt{2\chi_1/(\chi_1 + 1)} \simeq 1.1$ . Thus, the error in finding criterion (9) is expressed as  $\text{const} \cdot \exp(-\xi \gamma_0) < \text{const} \cdot \exp(-\xi/\eta_1) \simeq \text{const} \cdot \exp(-1.1 \xi)$ , and in physically real cases  $z \simeq 1$  (for the example from (1), we calculate  $z = 1.16$  and  $\gamma_0 = 1.49$ ) and the constant is also close to unity. Therefore even in the case  $L/\lambda \simeq 1$ , when the perturbation wavelength coincides with the thickness of the detonation zone, the error of the approximation in criterion (9) will be less than  $\exp(-2.2\pi) \simeq 0.1\%$ , which is quite admissible within the framework of the linear stability theory and the ideal-gas hypothesis.

Comparison of criterion (9) with that of Shchelkin<sup>1</sup> gives exact numerical agreement, thereby fully confirming the conclusions of<sup>1</sup> on the instability of a detonation wave in an ideal gas.

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

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