Gradient Relations at the Front of Detonation Waves in Gases

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The so-called gradient relations, i.e., analytical formulas that define the relationship between partial spatial derivatives (gradients) of pressure, density, and gas particle velocity behind a plane detonation front and the acceleration of the front, are obtained within the framework of a model based on the assumption of isothermality of gas detonation products. It is shown that the relations can be used to simplify the description of overdriven detonation regimes in chemically reacting gas.

Introduction. If the motion of the medium behind the front of the shock wave (the surface of strong discontinuity) is described by the smooth one-dimensional solution and the parameters ahead of the front are constant, it is possible to give a one-to-one correspondence between the partial spatial derivative (gradient) of any gas-dynamic parameter and the time derivative of the velocity (acceleration) of the front *dD/dt*. For one-dimensional adiabatic flow of perfect gas, such gradient relations at the front of the shock wave are presented in [1, 2].

In [3], it was possible to remove restrictions conditioned by the model of perfect gas by using the natural assumption on the notation form of the calorific equation of state (internal energy) of medium. The assumption is based on the fact that in view of the calorific equation of state, the total internal energy of gas $U = U_{th} + U_{ch}$ including the thermodynamic part U_{th} and the potential chemical energy U_{ch} may be written in the form of the function of pressure p and density ρ: $U = U(p, \rho)$. This relation is valid for both inert media and reaction products in the state of chemical equilibrium. By equilibrium flows of reacting gases one means such flows in which the velocity of reaching the chemical equilibrium much exceeds the velocity of change of the outer parameters, i.e., the chemical reaction can be regarded as instantaneous one. As a result, more universal gradient relations are also usable for the detonation front (strong discontinuity with heat release) with allowance for heat effect. Thus for the one-dimensional detonation wave (DW) propagating along the coordinate axis r, they have the form:

$$\left(\frac{\partial \rho}{\partial r}\right)_* = \frac{1}{M_*^2 - 1}\left\{\left[3(A+1) - A/M_*^2\right] \cdot \frac{\rho_* - \rho_0}{c_*^2} \cdot \frac{dD}{dt}\right\},$$
$$\left(\frac{\partial u}{\partial r}\right)_* = \frac{1}{M_*^2 - 1}\left\{\frac{\rho_0}{\rho_*} \cdot (2A+3) \cdot \frac{u_* - u_0}{c_*^2} \cdot \frac{dD}{dt}\right\}, \quad (1)$$

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$$\left(\frac{\partial p}{\partial r}\right)_* = \frac{1}{M_*^2 - 1}\left\{\frac{\rho_0}{\rho_*}\cdot\left[A + 2 + (A+1)/M_*^2\right]\cdot\frac{p_* - p_0}{c_*^2}\cdot\frac{dD}{dt}\right\}, \quad (1)$$

$$M_* = (D - u_*)/c_*,\ A = \frac{2 + (1/\rho_* - 1/\rho_0)/(U_p)_*}{(1/M_*)^2 - 1},\ U_p = \left(\partial U/\partial p\right)_\rho,$$

where D is the front velocity, u is the mass velocity, c is the equilibrium sound velocity, M is the Mach number of the relative flow; by low indices 0 and * we denote the parameter ahead of the front (in the initial state) and at the wave front, respectively. From (1), it follows that the gradients of gas-dynamic functions are proportional to the acceleration of the front dD/dt. Moreover, specific values of the proportionality coefficients are defined by the functional dependence $U = U(p, \rho)$ and D.

In the present work, the general formulas of gradient relations (1) are adapted for simplified description of propagation of overdriven detonation modes in a chemically reacting gas.

Isothermal Model of Detonation. Here is it assumed that for intensely explosive gas mixtures with chemical reaction temperature of about 2500–4000 K, the equilibrium adiabatic index is close to unity [4], i.e., detonation products (DP) are almost the isothermal medium and it is possible to consider that $p/\rho = const$. Similar behavior of DP may be interpreted by the strong dependence of heat effect on temperature. Thus, in [5], it is shown that due to the dissociation processes of gas molecules, the total internal energy of DP is close to the step function with a sharp rise of values at temperature of about 3000 K. Within the framework of this model, the gas-dynamic parameters at the detonation front may be explicitly expressed in terms of the velocity of front D, namely, the degree of DW overdriving

$$\alpha = D/D_{CJ}\,. \quad (2)$$

Hereinafter, the lower index "CJ" is used to denote the parameters of the stationary (steady) Chapman-Jouget detonation.

The isothermal model of detonation includes the following relations for the front of DW propagating in a motionless explosive gas ($u_0 = 0$):

$$\rho_*(D - u_*) = \rho_0 D,\ p_* + \rho_*(D - u_*)^2 = p_0 + \rho_0 D^2,\ p_*/\rho_* = c_{CJ}^2 = \text{const}, \quad (3)$$

where c_{CJ} is an equilibrium sound velocity in DP. If one completes equations (3) by the Chapmen-Jouget condition with respect to equilibrium sound velocity

$$c_{CJ} = D_{CJ} - u_{CJ}\,, \quad (4)$$

it is possible to estimate the values of DP parameters at the front of the Chapman-Jouget detonation assuming that the velocity of the front D_{CJ} is given.

Usually, for DW, $p_* >> p_0$ such that the initial pressure of the gas mixture may be neglected. Then, the solution of equations (3)-(4) yields

$$u_{CJ} = c_{CJ} = D_{CJ}/2,\quad \rho_{CJ} = 2\rho_0,\quad p_{CJ} = 2\rho_0 c_{CJ}^2\,. \quad (5)$$

By using these formulas, from relations (2) and (3) we obtain the dependences of dimensionless front parameters $\mathbf{Y}_* = \{p_*/p_{CJ}, \rho_*/\rho_{CJ}, u_*/u_{CJ}\}$ on the degree of overdriving α:

$$p_*/p_{CJ} = \rho_*/\rho_{CJ} = \alpha\left(\alpha + \sqrt{\alpha^2 - 1}\right),\ u_*/u_{CJ} = \alpha + \sqrt{\alpha^2 - 1}\,. \quad (6)$$

Note that in comparison with exact equilibrium calculations [4], the error of formulas (6) is small. For example, it is less than 3 % for $\alpha = 1.2$.

We demonstrate that the isothermal model is also well suited for the description of equilibrium flows of DP. For this purpose, consider the problem of the medium motion behind the front of the self-sustaining plane DW arisen at the coordinate origin (near the wall) at time $t = 0$ and propagating along the coordinate axis *r* with constant velocity D_{CJ}. According to [6], the solution of this problem

may be presented in the form of simple wave (the Riemann wave), which is defined by two ordinary differential equations and the relation between self-similar variable r/t, mass velocity u, and the sound velocity c:

$$dp = \rho c \cdot du, \quad d\rho = \rho / c \cdot du, \quad u + c = r/t \tag{7}$$

provided that at the front of DW, gas-dynamic parameters of DP correspond to the Chapman-Jouget state.

Figure 1 presents the numerical solution (solid lines) [7] of the considered problem in the form of the dependence of dimensionless parameters of DP $\mathbf{Y} = \{p/p_{CJ}, \rho/\rho_{CJ}, u/u_{CJ}\}$ on dimensionless variable r/r_*. This solution is obtained with allowance for the shift of the chemical equilibrium of DP. The calculations are performed at $p_0 = 0.1013$ MPa and $T_0 = 298.15$ K for the stoichiometric acetylene-oxygen mixture $C_2H_2 + 2.5O_2$ ($D_{CJ} = 2424$ m/s). This figure also shows the approximate solution (dashed lines) obtained in the form of analytic formulas in integrating (7) with allowance for equations (3)-(6):

$$\frac{u}{u_{CJ}} = \begin{cases} 2r/r_* - 1, & \text{for } 0.5 < r/r_* \le 1 \\ 0, & \text{for } 0 \le r/r_* \le 0.5 \end{cases}$$
$$\ln\frac{p}{p_{CJ}} = \ln\frac{\rho}{\rho_{CJ}} = \begin{cases} 2r/r_* - 2, & \text{for } 0.5 < r/r_* \le 1 \\ -1, & \text{for } 0 \le r/r_* \le 0.5 \end{cases} \tag{8}$$

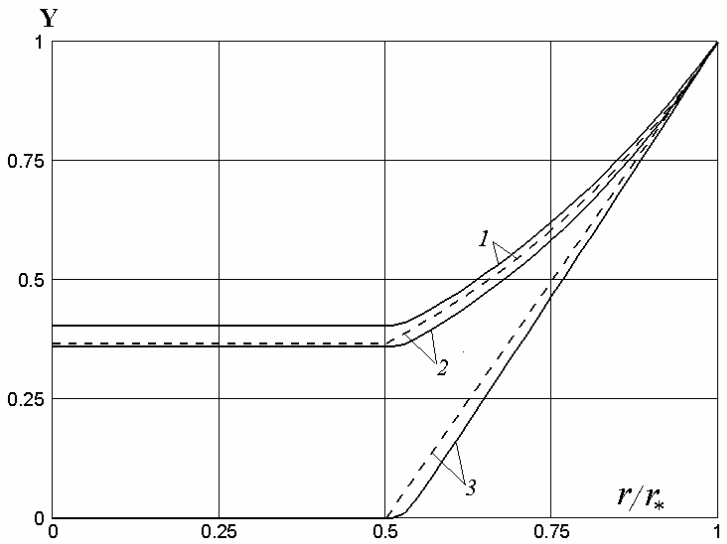

Fig. 1. Distribution of dimensionless DP parameters $\mathbf{Y}$ behind the front by the self-sustained plane DW: 1 – ρ/ρ_{CJ}, 2 – p/p_{CJ}, 3 – u/u_{CJ}, solid lines are the results of equilibrium calculations [7], dashed lines are the approximate solution (8).

It is obvious that solution (8) quite adequately approximates the results of numerical calculations [7] with relatively small error, which tends to zero in approximation to the DW front ($r/r_* \to 1$). In this connection, to describe the DW in gases in more simple way, the following approach, which is sufficiently universal, may be recommended.

Firstly, one calculates exact values of the velocity of front D_{CJ}^e and other equilibrium parameters $p_{CJ}^e, \rho_{CJ}^e, u_{CJ}^e$ (for example, according to technique [4]) or uses well-known results of similar calculations for a specific explosive mixture. All other calculations are performed according to the

approximate model (provided that the medium is isothermic behind the front) for the dimensionless parameters of DP $\mathbf{Y}$. Note that for the estimate of approximate values p_{CJ}, ρ_{CJ}, u_{CJ} as it is shown above, it is sufficient to specify only the front velocity (let $D_{CJ} = D_{CJ}^e$). Below, to obtain specific quantitative results, it is necessary to return to dimensional variables using exact values of equilibrium parameters p_{CJ}^e, ρ_{CJ}^e, u_{CJ}^e for the approximate solution to approximate the exact solution in the best way.

Gradient Relations and Simulation of Overdriven DW. Assuming the isothermality of DP when the conditions $p/\rho = \text{const}$ and $U_p = \infty$ hold, by using (2)-(6), it is possible to transform formulas (1) in the form

$$\begin{gathered}\frac{1}{p_{CJ}}\left(\frac{\partial p}{\partial r}\right)_* = \frac{1}{\rho_{CJ}}\left(\frac{\partial \rho}{\partial r}\right)_* = -\frac{3M_*^2+1}{2D_{CJ}M_*^4(\alpha^2-1)}\cdot\frac{d\alpha}{dt},\\ \frac{1}{u_{CJ}}\left(\frac{\partial u}{\partial r}\right)_* = -\frac{M_*^2+3}{2D_{CJ}M_*^2(\alpha^2-1)}\cdot\frac{1}{\alpha}\cdot\frac{d\alpha}{dt}, \quad M_* = \alpha-\sqrt{\alpha^2-1}.\end{gathered} \tag{9}$$

Thus, we have gradient relations at the front of gas detonation, which have the following structure:

$$\left(\partial\mathbf{Y}/\partial r\right)_* = \mathbf{F}(\alpha)\cdot d\alpha/dt,$$

where $\mathbf{F}(\alpha)$ is the explicit function of degree of overdriving. Moreover, in order to use these relations, it is sufficient to know only the dependence of current front position on time $r_* = r_*(t)$ as such dependence allows one to find the velocity $D = dr_*/dt$ and acceleration $dD/dt = d^2r_*/dt^2$ of the DW front and, hence, the values α and $d\alpha/dt$. In addition, by using formulas (6), it is easy to define other parameters at the front $\mathbf{Y}_*$.

This implies that knowing only the dependence $r_* = r_*(t)$, we can construct the approximate solution behind the DW front accurate to terms $o(h^2)$ for any given time t:

$$\mathbf{Y} = \mathbf{Y}_* - h\left(\partial\mathbf{Y}/\partial r\right)_* + o(h^2), \tag{10}$$

where $h = r_* - r$ is the distance from the front to the point with the coordinate r, at which the values of parameters of DP $\mathbf{Y}$ are defined. Similar solutions, as it is noted in [8], may be applied in interpretation of experimental data or investigation of approximation of numerical difference schemes near a moving boundary corresponding to the strong discontinuity.

It is known that the plane overdriven DW in gas reaches the Chapman-Jouget mode ($\alpha = 1$) at infinity without considering friction and heat-release losses. Here, the distribution of gas-dynamic parameters of DP behind the front in the limit corresponds to the solution of considered problem (7). This solution is described by formulas (8) in case of isothermality of DP.

Obtained gradient relations (9) allow one to establish the asymptotic law of propagation of overdriven DW sufficiently easy. Thus, on the one part, as $\alpha \to 1$, from (9) and the natural dependence $D = \alpha D_{CJ} = dr_*/dt$, it follows that

$$\frac{1}{u_{CJ}}\left(\frac{\partial u}{\partial r}\right)_* \approx -\frac{1}{\alpha-1}\cdot\frac{d\alpha}{dr_*}. \tag{11}$$

On the other part, as $r_* \to \infty$, from (8), it follows that

$$\frac{1}{u_{CJ}}\left(\frac{\partial u}{\partial r}\right)_* = \frac{2}{r_*}. \tag{12}$$

Comparing (11) with (12), we obtain the differential equation for finding the asymptotic law

$$\frac{2}{r_*} = -\frac{1}{\alpha - 1} \cdot \frac{d\alpha}{dr_*}.$$

After integrating, we find

$$(\alpha - 1) r_*^2 = r_0^2 \quad \text{or} \quad \left(\frac{1}{D_{CJ}} \cdot \frac{dr_*}{dt} - 1 \right) r_*^2 = r_0^2 \qquad (r_0 = \text{const}).$$

One more integration yields the asymptotic law of propagation of overdriven DW

$$D_{CJ}(t - t_0) = r_* \left(1 - r_0 / r_* \operatorname{arctg}(r_* / r_0)\right), \tag{13}$$

where t_0 is some constant. This law implies that in degenerating of the overdriven DW into the Chapman-Jouget wave, the coordinate of front $r_* = r_*(t)$ tends to the asymptote

$$r - D_{CJ} t = \text{const}.$$

It is essentially different from the behavior of the plane shock wave in degenerating it into acoustic one since the shock wave has no asymptote. Note that similar conclusions are firstly obtained in [9]. However, presented in [9], the asymptotic law

$$D_{CJ}(t - t_0) = r_* \left(1 + r_0^2 / r_*^2 + \cdots\right) \tag{14}$$

differs from (13). Deriving (14), one uses the assumption on chemical inertness of DP (the heat release occurs only at the detonation front).

Conclusions. Thus, we obtained gradient relations at the detonation front adapted for a simplified description of overdriven gas detonation. It is shown that these relations can be used in the construction of approximate solutions of nonstationary gas-dynamic problems.

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