Detonation As Combustion in a Supersonic Flow of a Combustible Mixture

A. A. Vasil'ev[a,b,*]

UDC 544.452+544.454

Abstract: The classical models of steady propagation of combustion and detonation waves in a combustible mixture describe the increase in the system entropy to a maximum value in the case of deflagration (subsonic) combustion of the mixture driven by slow processes of heat conduction and diffusion. In the detonation (supersonic) regime, however, where one of the leading roles belongs to the bow shock wave, the models predict that the combustible system after completion of the chemical reaction "chooses" the minimum increase in entropy. These predictions are inconsistent with the formulation of chemical thermodynamics that the entropy of the system reaches its maximum value after the spontaneous irreversible chemical reaction is finalized and the equilibrium state is established. It is shown in the present study that the predictions of the classical models on the minimum increase in entropy in the case of detonation are eliminated if detonation is considered as a process of combustion of a mixture preliminary subjected to an irreversible process of compression and heating of the initial mixture in the bow shock wave (chemical spike) with a corresponding increase in entropy of the initial mixture and subsequent energy release from the mixture in an irreversible process of mixture conversion to chemical reaction products.

Keywords: combustion, detonation, irreversible processes, increase in entropy, chemical equilibrium of products, chemical energy release in subsonic and supersonic flows.

DOI: 10.1134/S0010508222060077

INTRODUCTION

Idealized classical models of detonation with a plane front proposed at the end of the 19th century by Michelson, Chapman, and Jouguet, which were later developed by Grib, Zel'dovich, Neumann, and Döring, are still used for estimating the velocity and other parameters, despite the modern concepts of the non-classical detonation wave structure treated as a complicated gas-dynamic complex consisting of compression and rarefaction waves, shock wave configurations of regular and Mach types, transverse waves, induction and reaction regions with parameters inhomogeneously distributed in time and space, etc. The main postulates of these models are widely presented in scientific and educational literature and are well known to specialists (see, e.g., [1–3]).

One of the main conclusions from these theories is the existence of two steady (self-sustained) regimes of propagation: detonation (with a supersonic velocity) and deflagration (with a subsonic velocity). These regimes are determined by the points of tangency of the Michelson–Rayleigh straight lines (geometric analog of the mass and momentum conservation law) with the energy release adiabat (analog of the energy conservation law—Hugoniot curve). The chemical reaction at the tangency points is assumed to be finalized, and the main gas-dynamic and chemical parameters are assumed to reach their steady values. For the entropy of combustion and detonation products, this testifies to the existence of an extreme point, i.e.,

[a]Lavrentyev Institute of Hydrodynamics, Siberian Branch, Russian Academy of Sciences, Novosibirsk, 630090 Russia, [*]gasdet@hydro.nsc.ru.
[b]Novosibirsk State University, Novosibirsk, 630090 Russia.

the contact of the Michelson–Rayleigh straight line with the Hugoniot curve occurs simultaneously with the contact of these lines with the constant-entropy curve (Poisson's adiabat). According to the classical theories, the constant-entropy line $S_d = $ const touches the energy release adiabat at the detonation point [with respect to the initial state of the mixture (point O) marked by the subscript d] from below; at the deflagration point (marked by the subscript df), the line $S_{df} = $ const touches the energy release adiabat from above. This means that the entropy of combustion products in the subsonic region (where the constant-entropy line touches the Hugoniot curve from above) is characterized by an extreme point with the maximum value. However, the situation with the contact point in the supersonic region is different: the constant-entropy line touching the Hugoniot curve from below is characterized by an extreme point with the minimum value; moreover, $S_d < S_{df}$. In other words, one of the conclusions of the classical theories is the fact that, in contrast to combustion, the system in the case of detonation "chooses" the regime of propagation with the minimum increase in entropy. It is worth noting that the authors of the classical detonation theories paid attention to this fact in their studies, but did not analyze it in detail. The question why detonation "chooses" the regime with the smallest increase in entropy is still open. In chemical thermodynamics, the increase in entropy serves as a criterion of the direction of irreversible chemical reactions; moreover, when the reaction is finalized and the equilibrium state is reached, the entropy of the combustible mixture has to reach the maximum value, $S = S_{\max}$. When the equilibrium state is reached, the corresponding thermodynamic potentials (internal energy, enthalpy, and Gibbs and Helmholtz energies) become constant: $(dU)_{S,V} = 0$, $(dH)_{S,P} = 0$, $(dA)_{T,V} = 0$, and $(dG)_{T,P} = 0$, while the potentials themselves reach the minimum values: $U = U_{\min}$, $H = H_{\min}$, $A = A_{\min}$, and $G = G_{\min}$ [4].

The estimated conclusion on smaller irreversible losses in the case of detonation as compared to the combustion processes aroused much excitement many years later, during the development of new-generation engines operating in regimes of detonation burning of combustible mixtures. Many experimental results on this topic were obtained, hundreds of papers were published, but the question about the efficiency is still open. This fact serves as an additional argument for considering this problem.

In the present study, we made an attempt to clarify the issue of the increase in entropy in the cases of combustion and detonation and of the relationship between the entropy values in irreversible processes, i.e., shock wave action on the combustible mixture and chemical reactions. Special attention should be paid to the fact that the chemical reaction in the classical models of combustion and detonation is postulated to be finalized at the tangency points!

For better presentation of the material, the author has to describe briefly the fundamentals of the classical theories that describe propagation of processes with chemical reactions and to use necessary formulas.

IDEALIZED ONE-DIMENSIONAL MODELS OF COMBUSTION AND DETONATION

The classical one-dimensional theory of combustion and detonation is based on the mass, momentum, and energy conservation laws written in the coordinate system of the motionless wave front for a constant-section flow tube:

$$\rho_0 w_0 = \rho w, \qquad P_0 + \rho_0 w_0^2 = P + \rho w^2,$$

$$H_0 + w_0^2/2 = H + w^2/2 + Q.$$

Here w_0 and w are the velocities of the flow entering and leaving the wave front, $V = 1/\rho$ is the specific volume of one mole per unit mass (a quantity inverse to the density of the mixture ρ), P is the pressure, H is the enthalpy, and Q is the specific energy release of the mixture (see, e.g., [1, 2]); the parameters in the initial state are denoted by the zero subscript.

The first two equations yield

$$\frac{P - P_0}{V - V_0} = -\rho_0^2 w_0^2 = \text{const},$$

i.e., the equation of the straight line in the plane (P, V), which is called the Michelson–Rayleigh straight line. From this equation, one can derive two useful relations for the velocities:

$$w_0^2 = V_0^2 \frac{P - P_0}{V_0 - V}, \quad w^2 = V^2 \frac{P - P_0}{V_0 - V};$$

being substituted into the energy equation, these relations allow one to obtain several auxiliary formulas for the enthalpy H and internal energy U:

$$H - (H_0 + Q) = (w_0^2 - w^2)/2$$

$$= (P - P_0)(V_0 + V)/2,$$

$$U - (U_0 + Q) = (w_0^2 - w^2)/2 + P_0 V_0 - PV$$

$$= (P + P_0)(V_0 - V)/2.$$

Within the framework of the ideal gas model with the equation

$$P = \rho RT = RT/V$$

the enthalpy is expressed by the formula

$$H = U + PV = \frac{\gamma}{\gamma - 1} PV$$

(γ is the ratio of specific heats); therefore, the energy equation (for H or U) takes the form $P = F(V, Q)$. This function is called the energy release adiabat (or Hugoniot adiabat):

$$\frac{P}{P_0}\left(\frac{V}{V_0}\frac{\gamma + 1}{\gamma - 1} - 1\right) = \frac{\gamma + 1}{\gamma - 1} - \frac{V}{V_0} + 2\frac{Q}{P_0 V_0}.$$

After transformations, this function turns into the hyperbola equation

$$\left(\frac{P}{P_0} + \frac{\gamma - 1}{\gamma + 1}\right)\left(\frac{V}{V_0} - \frac{\gamma - 1}{\gamma + 1}\right)$$
$$= 1 - \left(\frac{\gamma - 1}{\gamma + 1}\right)^2 + 2\frac{\gamma - 1}{\gamma + 1}\frac{Q}{P_0 V_0}.$$

At $Q = 0$, we obtain the shock adiabat equation

$$\left(\frac{P}{P_0} + \frac{\gamma - 1}{\gamma + 1}\right)\left(\frac{V}{V_0} - \frac{\gamma - 1}{\gamma + 1}\right)$$
$$= 1 - \left(\frac{\gamma - 1}{\gamma + 1}\right)^2 = \text{const}.$$

It should be particularly noted that the shock adiabat and the Hugoniot adiabat form a geometric area of points of states behind the shock wave (SW) and in reaction products with the energy release Q, respectively.

BASIC CONCLUSIONS
OF IDEALIZED MODELS

The lines $P = P_0 = \text{const}$ and $V = V_0 = \text{const}$ divide the (P, V) plane into four quadrants (Fig. 1): nonphysical quadrants I and III, supersonic quadrant II, and subsonic quadrant IV. The energy release adiabat as a hyperbola is shifted with respect to the initial state O so that the point O lies outside the hyperbola. The shock adiabat is also a hyperbola, but it passes through the initial point. Many curves can be drawn from the point O to the energy release adiabat as a hyperbola. There are three variants of the mutual position of the energy release adiabat and the straight line: (a) no intersection; (b) intersection at two points; (c) tangent contact of the straight line and adiabat.

Let us introduce the dimensionless variables

$$y = \frac{P}{P_0}, \quad x = \frac{V}{V_0}, \quad q = \frac{Q}{\gamma P_0 V_0} = \frac{Q}{c_0^2},$$
$$\eta = \frac{\gamma - 1}{\gamma + 1}, \quad \mathrm{M}_0 = \frac{w_0}{c_0}.$$
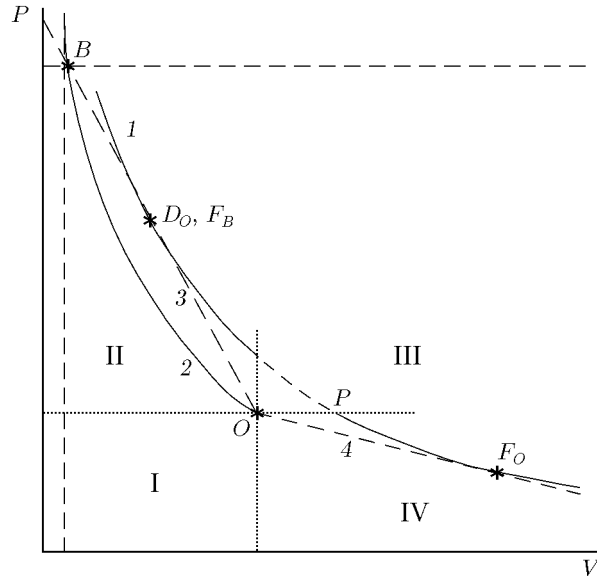

Fig. 1. Typical (P, V) diagram of the combustible mixture.

Then, the equation of the Michelson–Rayleigh straight line can be presented as

$$\frac{y - 1}{x - 1} = -\frac{w_0^2}{P_0 V_0} = -\gamma\frac{w_0^2}{c_0^2} = -\gamma\mathrm{M}_0^2.$$

The right side is always negative: the slope of the Michelson–Rayleigh straight lines is

$$\left(\frac{dy}{dx}\right)_{\mathrm{MR}} = -\gamma\mathrm{M}_0^2 = -\frac{y - 1}{1 - x};$$

the left side is negative if the following conditions are simultaneously satisfied:

(a) $y > 1$ ($P > P_0$), $x < 1$ ($V < V_0$) (see quadrant II for supersonic detonation processes in Fig. 1);

(b) $y < 1$ ($P < P_0$), $x > 1$ ($V > V_0$) (see quadrant IV for subsonic combustion processes in Fig. 1).

Condition (a) corresponds to compression of the medium with an increase in pressure; condition (b) refers to expansion of the medium with a decrease in pressure. Figure 1 shows a typical plot of the states of the combustible system and its products: initial state O, energy release adiabat (Hugoniot) *1*, shock adiabat *2*, and Michelson–Rayleigh straight lines *3* and *4* touching the Hugoniot curve *1* at the points D_O (self-sustained detonation, quadrant II) and F_O (self-sustained deflagration, quadrant IV). Lines *1–4* are constructed with respect to initial point O.

In the quadrant $P > P_0$, $V < V_0$, the Hugoniot adiabat describes the final states of supersonic regimes of detonation propagation; in the quadrant $P < P_0$, $V > V_0$, it describes the state of subsonic regimes of deflagration combustion, including the normal combustion

regime. The Michelson–Rayleigh straight lines for the detonation quadrant (from the initial state point O), in addition to the final states with partial energy release of the mixture and final energy release on the Hugoniot curve, describe the set of states of the initial mixture behind the SWs propagating with different (supersonic) velocities. For example, see the point B on the shock adiabat being intersected by the Michelson–Rayleigh straight line (see Fig. 1). The shock adiabat in the dimensionless variables has the form $(y+\eta)(x-\eta) = 1-\eta^2$ or is presented by the formula

$$y = \frac{1-\eta x}{x-\eta} = \frac{(\gamma+1)-(\gamma-1)x}{(\gamma+1)x-(\gamma-1)}.$$

The first law of the classical thermodynamics (nonreacting flows) is formulated as $\delta Q = dU + P \cdot dV = T \cdot dS$, and the second law is expressed as $\Delta S \geqslant 0$. Here δQ is the heat supplied to the system, dU is the change in the internal energy of the system (one of the thermodynamic potentials), $P \cdot dV$ is the work performed by the system, T is the temperature, and dS is the entropy differential. For a closed system, we have $\delta Q = 0$, and $S = \text{const}$ is an adiabatic process. The form of the adiabat equation (called Poisson's adiabat) for an ideal gas is obtained from the conditions $dS = 0$ and $dU + P \cdot dV = c_v dT + RT \cdot dV/V = 0$. Using the relations $c_p - c_v = R$ and $\gamma = c_p/c_v$ (where c_p and c_v are the specific heats at constant pressure and volume, respectively) for an ideal gas, we obtain the equation of the adiabatic process $PV^\gamma = \text{const}$ ($TV^{\gamma-1} = \text{const}$ and $PT^{-\gamma/(\gamma-1)} = \text{const}$) in the dimensionless form: $yx^\gamma = \text{const}$. It should be specially noted that this formula is an equation of a reversible process, in contrast to the shock (and Hugoniot) adiabat as a set of discrete points of final states not connected with each other by the cause-and-effect relationship.

The velocity of sound is determined by the derivative of the Poisson's adiabat equation

$$c^2 = \left(\frac{dP}{d\rho}\right)_S = \frac{\gamma P}{\rho}.$$

At the initial point O, we have

$$c_0^2 = \left(\frac{dP}{d\rho}\right)_S \approx \left(\frac{P-P_0}{\rho-\rho_0}\right)_S.$$

The velocity of sound on the shock adiabat is determined by the relation

$$c^2 = \left(\frac{dP}{d\rho}\right)_{\text{SW}} = -\left(\frac{P_0 V^2}{V_0}\right)\left(\frac{dy}{dx}\right)_{\text{SW}}.$$

At the initial point O, we have

$$\left(\frac{dy}{dx}\right)_{\text{SW}} \to -\gamma,$$

$$c^2 = \left(\left(\frac{dP}{d\rho}\right)_{\text{SW}}\right)_O = \left(\left(\frac{dP}{d\rho}\right)_S\right)_O = c_0^2,$$

i.e., the slope of the classical Poisson's adiabat coincides with the slope of the shock adiabat: these lines are seen to be tangent to each other.

The equation of the energy release (Hugoniot) adiabat in the dimensionless variables is written as $y = (1 - \eta x + 2\eta\gamma q)/(x - \eta)$. From this equation, we can derive the coordinates of two important points corresponding to the combustion regime at $P = P_0 = \text{const}$ and to an instantaneous explosion of the mixture in a bomb at $V = V_0 = \text{const}$. If $P = P_0 = \text{const}$ ($y = 1$), the final state of the products is reached at $x_p = 1 + 2\eta\gamma q/(1+\eta) = 1 + (\gamma-1)q$; if $V = V_0 = \text{const}$ ($x = 1$), the final state is reached at $y_V = 1 + 2\eta\gamma q/(1-\eta) = 1 + \gamma(\gamma-1)q$.

If the initial mixture is at rest, then the mass conservation equation $\rho_0 D = \rho(D - u)$ yields a very important relation for the gas flow velocity behind the front: $u = D(1 - \rho_0/\rho)$. It is seen from this relation that, in the case of gas compression ($\rho_0/\rho = V/V_0 < 1$), the flow behind the shock front of the detonation wave (DW) moves in the same direction as the DW front ($u/D > 0$); at $\rho_0/\rho = V/V_0 > 1$ (expansion of combustion products), the gas flow direction is opposite to the direction of the combustion wave front velocity ($u/D < 0$). For the same case, the momentum conservation equation $P_0 + \rho_0 D^2 = P + \rho(D-u)^2 = P + \rho_0 D^2 - \rho_0 uD$ is transformed to $P = P_0 + \rho uD$, from which it follows that the pressure in the combustion wave decreases in the course of the chemical reaction ($u/D < 0$), and the pressure gradient, which makes the gas move and acquire a certain velocity, is directed upstream from the flame front, to the opposite side of the flame front velocity direction. Figure 2a shows idealized schemes of one-dimensional DW front structures, where 0 is the initial mixture, 1 is the bow front of the DW, i.e., the SW, 2 is the induction zone, 3 is the chemical reaction zone, and 4 is the region of detonation products. Figure 2b shows combustion front, where 1 is the initial mixture, 2 is the heating region, 3 is the chemical reaction region, and 4 is the region of combustion products. In the case of detonation (Fig. 2a), the particle velocity u in all regions follows the bow SW 1. In the case of combustion driven by the low-velocity processes of heat conduction and diffusion (from hot reaction products upstream to the combustible mixture), the combustion products move to the side opposite to the direction of flame front motion (Fig. 2b). It should be specially noted that the flame propagation velocities are determined with respect to the quiescent initial mixture.

Information about the tangency points of the Michelson–Rayleigh straight lines and the energy release adiabat can be extracted from the analysis of the adjoint system of conservation laws:
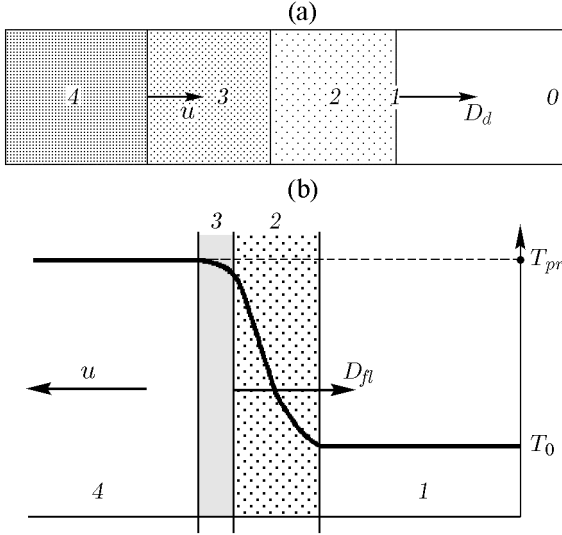
Fig. 2. Idealized structures of the DW (a) and combustion wave (b).

$$y_{MR} = (1 + \gamma M_0^2) - \gamma M_0^2 x,$$

$$y_H = \frac{1 - \eta x + 2\eta\gamma q}{x - \eta}.$$

Equating the right sides of the equations and applying some transformations, we obtain a quadratic equation of the classical form $ax^2 + bx + c = 0$ with the roots $x_{1,2} = [-b \pm \sqrt{b^2 - 4ac}]/2a$ (in this case, c is a coefficient that has nothing to do with the velocity of sound introduced above). Here $a = \gamma M_0^2$, $b = -(1 + \eta)(1 + \gamma M_0^2)$, and $c = 1 + (1 + \gamma M_0^2 + 2\gamma q)\eta$. Depending on the radicand, three cases are possible: (1) for $b^2 - 4ac < 0$, there are no real solutions (the Michelson–Rayleigh straight line has no intersection points with the energy release adiabat); (2) for $b^2 - 4ac > 0$, there are two solutions with the relations between them expressed by the Vieta formulas $x_1 + x_2 = -b/a$, $x_1 x_2 = c/a$ (the straight line intersects the Hugoniot curve at two points); (3) for $b^2 - 4ac = 0$, we have $x_1 = x_2 = -b/2a$ (the straight line and the Hugoniot curve touch each other). The equality of the radicand at the tangency point to zero yields an additional relation between the mixture parameters:

$$(1 + \eta)^2 (1 + \gamma M_0^2)^2$$
$$- 4\gamma M_0^2 \{(1 + \gamma M_0^2 + 2\gamma q)\eta + 1\} = 0.$$

This relation is first transformed to

$$\gamma^2 (1 - \eta)^2 M_0^4$$
$$- 2\gamma M_0^2 \{1 - \eta^2 + 4\eta\gamma q\} + (1 + \eta)^2 = 0,$$

and then to

$$M_0^4 - 2M_0^2 \{1 + q(\gamma^2 - 1)\} + 1 = 0.$$

The solutions of this equation are

$$(M_0^2)_{1,2} = \{1 + q(\gamma^2 - 1)\}$$
$$\pm \sqrt{\{1 + q(\gamma^2 - 1)\}^2 - 1}.$$

From here, we derive an important relation between the Mach numbers at the detonation and deflagration tangency points

$$(M_0)_1 (M_0)_2 = (M_0)_d (M_0)_{df} = 1$$

or between the detonation and deflagration velocities $D_d D_{df} = c_0^2$. Usually, $q \gg 1$; therefore, the Mach number for detonation (with the plus sign at the root) is

$$(M_0^2)_d \approx 2(\gamma^2 - 1)q$$

or $D_{0d} \approx \sqrt{2(\gamma^2 - 1)Q}$, and the Mach number for deflagration (with the minus sign at the root) is

$$(M_0^2)_{df} \approx 0.5/[(\gamma^2 - 1)q]$$

or $D_{0df} \approx 1/\sqrt{2(\gamma^2 - 1)Q}$. It is seen from this formulas that an increase in Q leads to an increase in the detonation velocity and to a decrease in the deflagration velocity.

At the tangency point of the detonation branch of the Hugoniot curve, we have

$$x_{*d} = -b/2a = (1 + \eta)(1 + \gamma M_{0d}^2)/2\gamma M_{0d}^2$$
$$= (1 + \gamma M_{0d}^2)/[(\gamma + 1)M_{0d}^2] \approx \gamma/(\gamma + 1),$$

$$y_{*d} = 1 + \gamma M_{0d}^2 (1 - x_{*d}) = (\gamma M_{0d}^2 + 1)/(\gamma + 1)$$
$$= x_{*d} M_{0d}^2 \approx \gamma M_{0d}^2/(\gamma + 1).$$

As, for the specified velocity at the bow shock front of the DW, we have $y_{SW} = [2\gamma M_{0d}^2 - (\gamma - 1)]/(\gamma + 1) \approx 2\gamma M_{0d}^2/(\gamma + 1)$, then, $y_{SW} \approx 2y_{*d}$, i.e., the pressure of detonation products is approximately one half of the pressure at the front of the SW moving with the same velocity. At the tangency point of the Hugoniot curve and the deflagration branch, we have to use the deflagration Mach number $M_{0df} = 1/M_{0d} \ll 1$ in the formula for x_{*df}; then,

$$x_{*df} = -b/2a = (1 + \eta)(1 + \gamma M_{0df}^2)/2\gamma M_{0df}^2$$
$$= (1 + \gamma M_{0df}^2)/[(\gamma + 1)M_{0df}^2]$$
$$\approx 1/[(\gamma + 1)M_{0df}^2] \approx 2(\gamma - 1)q,$$

$$y_{*df} = 1 + \gamma M_{0df}^2 (1 - x_{*df})$$
$$= (\gamma M_{0df}^2 + 1)/(\gamma + 1) = x_{*df} M_{0df}^2 \approx 1/(\gamma + 1).$$

The velocity of sound in reaction products at the tangency points coincides with the velocity of the exhausting flow of the products with respect to the wave front:

$$w = c: \quad c^2 = \left(\frac{dP}{d\rho}\right)_S = \frac{\gamma P}{\rho}$$

$$= \frac{-P_0 V^2}{V_0}\left(\frac{dy}{dx}\right)_S = \gamma P_0 V_0 M_0^2 \left(\frac{V^2}{V_0^2}\right)$$

$$= \frac{w_0^2 V^2}{V_0^2} = w^2$$

(for both detonation and deflagration). In other words, the velocity of the flow of reaction products with respect to the front is equal to the local velocity of sound and $M = w/c = 1$ (sonic exhaustion). This is the famous Chapman–Jouguet condition, which is also known in the form $D = u + c$.

CHANGE IN ENTROPY DUE TO COMBUSTION AND DETONATION

In chemical thermodynamics, the internal energy as one of thermodynamic potentials (and also the enthalpy and the Gibbs and Helmholtz potentials) is supplemented with an additional chemical potential characterizing the change in the number of moles:

$$dU = T \cdot dS - P \cdot dV + \sum_i \mu_i \, dn_i$$

(μ and n are the chemical potential and the number of moles of the specified chemical species, respectively).

As the tangency points characterize a steady process of propagation with a finalized chemical reaction, the final composition is further assumed to stay unchanged ($dn_i = 0$); therefore, the last sum can be neglected. Then, we can write $dS = \dfrac{c_v \, dT}{T} + \dfrac{R \, dV}{V}$; after integration (in the case with the initial state at the point O), we obtain

$$\frac{S - S_0}{R} = \ln\left(\frac{T^{1/(\gamma-1)}V}{T_0^{1/(\gamma-1)}V_0}\right)$$

$$= \frac{1}{(\gamma-1)\ln(yx^\gamma)} = \frac{\hat{S}(y, x)}{\gamma - 1}.$$

This is the basic formula for estimating the changes in the entropy of reaction products with respect to the initial mixture and also for the change in the entropy on the shock adiabat. The first derivative of the entropy function is

$$\frac{d\hat{S}}{dx} = \frac{1}{yx^\gamma}[y'x^\gamma + y\gamma x^{\gamma-1}] = \frac{y'}{y} + \frac{\gamma}{x}.$$

Here the second term is a positive number, and the first one is a negative number because $y' = [(1 - \eta x + 2\eta\gamma q)/(x - \eta)]' = -(1 - \eta^2 + 2\eta\gamma q)/(x - \eta)^2 < 0$.

The sign-variable expression for $\dfrac{d\hat{S}}{dx}$ can be equal to zero, which would testify to the existence of an extreme point. To find this point, we solve the equation

$$\frac{d\hat{S}}{dx} = \frac{-1}{x - \eta} - \frac{\eta}{1 - \eta x + 2\eta\gamma q} + \frac{\gamma}{x} = 0.$$

This formula can be transformed to a quadratic equation of the classical form $ax^2 + bx + c = 0$ with the roots $x_{1,2} = [-b \pm \sqrt{b^2 - 4ac}]/2a$, where $a = \gamma > 0$, $b = -(\gamma + 1)(1 + \eta + 2\eta\gamma q) = -2\gamma[1 + (\gamma - 1)q] < 0$, and $c = \gamma(1 + 2\gamma\eta q) > 0$. As $q \gg 1$, then $x \approx (\gamma - 1)q \pm (\gamma - 1)q \cdot [1 - 2\gamma\eta q/(\gamma - 1)^2 q^2]^{1/2} \approx (\gamma-1)q \pm (\gamma-1)q \cdot [1 - \gamma/(\gamma^2 - 1)q]$, whence it follows that $x_+ \approx 2(\gamma - 1)q = x_{df}$ and $x_- \approx \gamma/(\gamma + 1) = x_d$, which coincide with the coordinates of the tangency point for deflagration (plus sign) and detonation (minus sign).

It is of interest to consider the behavior of the entropy function $\hat{S}$ along the Michelson–Rayleigh straight line $y = 1 - \gamma M^2(x - 1)$, i.e., in the case of a chemical reaction proceeding from the beginning (point O) to the end in steady detonation waves (point D_O) and deflagration waves (point F_O). The first derivative is

$$\frac{d\hat{S}}{dx} = \frac{y'}{y} + \frac{\gamma}{x} = -\frac{\gamma M^2}{1 - \gamma M^2(x - 1)} + \frac{\gamma}{x}$$

$$= \frac{-\gamma M^2 x + \gamma[1 - \gamma M^2(x - 1)]}{x[1 - \gamma M^2(x - 1)]}.$$

The numerator vanishes at $x = (1 + \gamma M^2)/[(\gamma + 1)M^2]$. For the detonation quadrant, we have $M^2 \gg 1$; therefore, the extreme point of the entropy is reached at $x \approx \gamma/(\gamma+1) = x_D$. For the subsonic quadrant, we have $M^2 \ll 1$; therefore, the extreme point of the entropy is reached at $x \approx 1/[(\gamma + 1)M^2] = x_{df}$. It should be emphasized that the initial state in these cases is at the point O, and the state of the products during the reaction is shifted from the point of the initial state to the extreme point (to the point D_O or F_O). The character of the extreme point is determined by the sign of the second derivative:

$$\frac{d^2\hat{S}}{dx^2} = \frac{\gamma^2 M^4}{[1 - \gamma M^2(x - 1)]^2} - \frac{\gamma}{x^2}$$

$$= \frac{\gamma^2 M^4 x^2 - \gamma[1 - \gamma M^2(x - 1)]^2}{x^2[1 - \gamma M^2(x - 1)]^2}.$$

For the detonation quadrant ($M^2 \gg 1$), we have

$$\frac{d^2\hat{S}}{dx^2} \approx \gamma^2 M^4[x^2 + (x - 1)^2] > 0,$$

i.e., the extreme point is a minimum point. For the deflagration quadrant ($M^2 \ll 1$), we have

$$\frac{d^2\hat{S}}{dx^2} \approx -\frac{\gamma}{x^2} < 0,$$

which means that the extreme point is a maximum point.

It should be specially noted that the system from the state O definitely arrives in a unique manner at the point F_O as a result of the chemical reaction by passing down along the deflagration Michelson–Rayleigh straight line with increasing temperature and decreasing pressure. These features were confirmed experimentally. However, there are two options of system arrival at the point D_O: from the point O along the detonation Michelson–Rayleigh straight line with a gradual increase in temperature and pressure and from the point O first to the point B of the chemical spike, and then from the point B along the same detonation Michelson–Rayleigh straight line to the point D_O with an increase in temperature and a decrease in pressure. For detonation, the change in entropy along the first path can be quantified (which was made by the authors of the classical theories), but there are absolutely no experimental verifications of the fact. However, there are many experimental facts confirming that the reaction in the DW "starts" from the state B in the chemical spike behind the bow shock of the DW rather than from the point O (this issue is discussed below).

Along Poisson's adiabat drawn from the initial point O, we have $PV^\gamma = P_0 V_0^\gamma$ (or $yx^\gamma = 1$ is a "hyperbola"); then, $S - S_0 = \dfrac{R}{\gamma - 1} \ln 1 = 0$.

The entropy on the shock adiabat increases as compared to the initial value owing to the process irreversibility:

$$\frac{S - S_0}{R} = \frac{1}{\gamma - 1} \ln(yx^\gamma) = \frac{1}{\gamma - 1} \ln\left[\frac{1 - \eta x}{x - \eta} x^\gamma\right].$$

At the initial point O, the shock adiabat ($y = (1 - \eta x)/(x - \eta)$) and Poisson's adiabat ($y = 1/x^\gamma$) have a tangency contact of the third order. The entropy on the energy release adiabat is also higher than the initial value.

Figure 3 shows the locations of the Michelson–Rayleigh straight line 1, energy release adiabat 3, and constant entropy line 2 for the case where the DW propagates with the minimum velocity with respect to the state O. The entropy has the minimum value at the tangency point on the detonation branch and increases with increasing Mach number; moreover, this situation is observed for both the overdriven and weak detonation regions. All points of the detonation branch 3 lie higher than the isentrope 2 drawn through the tangency point.

On the deflagration branch, the Mach number increases when passing from the normal flame to the regimes of transformation of laminar to turbulent burning and approaching the tangency point. Therefore, the entropy at the tangency point has the maximum value
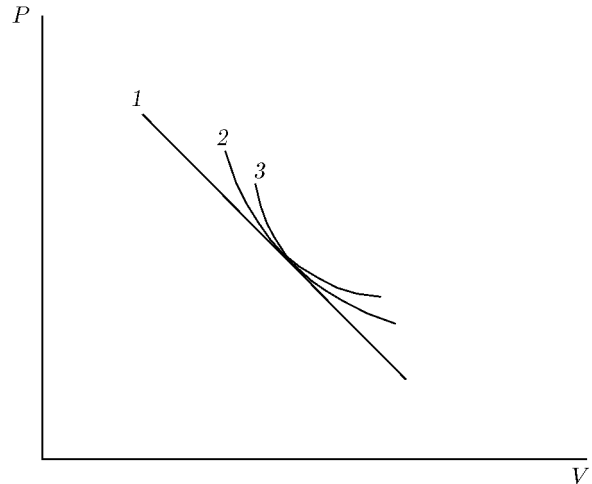
Fig. 3. Pattern of mutual tangency of the characteristic lines in the cases of deflagration and detonation.

among all points of the deflagration branch, i.e., for deflagration combustion, the energy release adiabat is curve 2 in Fig. 3, and the isentrope with the maximum value is curve 3. In other words, with respect to the initial state at the point O, the isentrope and the energy release adiabat change their places at the tangency points.

In the classical models, the condition $Q = \text{const}$ allows comparatively simple derivation of simple relations for the basic gas-dynamic parameters of detonation and deflagration. At the moment, almost all currently existing numerical programs use the condition $Q = Q(P, T)$ under the assumption of chemical equilibrium of chemical reaction products. The calculated values of the basic entropy factor yx^γ for typical regimes of the reaction in reacting mixtures of hydrogen and typical hydrocarbons with single (methane), double (ethylene), and triple (acetylene) chemical bonds being mixed with oxygen and air are summarized in Table 1. The second column of the table provides data for the characteristic points with respect to the initial state at the point O (see Fig. 1). The points D_d and D_{df} correspond to the tangency points for detonation and deflagration combustion (points D_O and F_O in Fig. 1), the point P refers to combustion at constant pressure (which almost coincides with the normal burning conditions), the point V corresponds to the regime of an instantaneous explosion in constant volume, and the point B is the chemical spike of the DW.

It is seen from Table 1 that, with respect to point O, the entropy factor yx^γ (last column) in reaction products has the minimum values for the detonation process and the maximum values for deflagration combustion. It should be emphasized that the formal

Table 1

Mixture	Characteristic points	y	x	γ	yx^γ	Mixture	Characteristic points	y	x	γ	yx^γ
$2H_2 + O_2$	B	33	0.18	1.32	3.44	H_2-air	B	27.64	0.19	1.32	3
	D_d	18.79	0.54	1.22	8.93		D_d	15.58	0.55	1.17	7.79
	V	9.59	1	1.21	9.59		V	8	1	1.18	8
	P	1	8.35	1.2	12.66		P	1	6.87	1.18	9.74
	D_{df}	0.49	16.07	1.19	13.23		D_{df}	0.48	13.09	1.2	10.38
$CH_4 + 2O_2$	B	55.49	0.11	1.17	4.39	CH_4–air	B	31.32	0.16	1.26	3.2
	D_d	29.32	0.54	1.21	13.88		D_d	17.17	0.55	1.18	8.57
	V	14.84	1	1.2	14.84		V	8.79	1	1.18	8.79
	P	1	12.7	1.19	20.41		P	1	7.52	1.19	10.99
	D_{df}	0.49	24.48	1.18	21.23		D_{df}	0.47	14.55	1.21	11.89
$C_2H_4 + 3O_2$	B	63.96	0.11	1.17	4.7	C_2H_4–air	B	33.48	0.16	1.26	3.32
	D_d	33.43	0.54	1.23	15.61		D_d	18.35	0.55	1.17	9.13
	V	16.87	1	1.22	16.87		V	9.38	1	1.17	9.38
	P	1	14.25	1.21	24.73		P	1	8.05	1.17	11.5
	D_{df}	0.48	27.96	1.2	26.08		D_{df}	0.48	15.43	1.18	12.16
$C_2H_2 + 2.5O_2$	B	64.57	0.11	1.19	4.87	C_2H_2–air	B	34.76	0.16	1.27	3.42
	D_d	33.83	0.54	1.26	15.64		D_d	19.11	0.55	1.17	9.48
	V	17.07	1	1.25	17.07		V	9.77	1	1.17	9.77
	P	1	14.2	1.23	26.23		P	1	8.4	1.16	11.78
	D_{df}	0.48	27.77	1.22	27.97		D_{df}	0.48	16.25	1.16	12.22

possibility of the regime with a transition from point O along the Michelson–Rayleigh straight line to the detonation state D_d from below with increasing pressure was not observed in experiments.

DETONATION AS COMBUSTION IN THE FLOW. BASIC RESULTS

Back in 1963, Shchelkin and Troshin [2] put forward an idea that detonation can be formally presented as deflagration with respect to the state behind the bow shock front of the DW. This presentation follows from the fact that the point B (the so-called Neumann spike of the DW) lies on the intersection of the shock adiabat *2* and the Michelson–Rayleigh straight line *3* emanating from the point O (see Fig. 1). In Fig. 1, with the state O being replaced by the state B (subscripts in the point notations), shows an additional quadrant,

which is a deflagration quadrant with respect to the state at the point B. The detonation point with respect to the initial state at O with a supersonic velocity D_O is simultaneously a subsonic deflagration point F_B with respect to the state B. In the steady wave, the formal transition from O to B with increasing pressure in the DW or from B downward with decreasing pressure in the deflagration combustion wave is not forbidden, though the states O and B are significantly different.

In the classical models, energy release is assumed to be independent of pressure and temperature: $Q = \text{const} \neq Q(P, T, V)$, though the majority of computations of combustion and detonation parameters are currently performed under a physically grounded assumption about chemical equilibrium of the products. The calculated coordinates of the characteristic points x_i for various oxygen and air mixtures and for basic regimes for two states (initial system O) and system with the parameters of state behind the bow SW front of the detonation front (Neumann spike) B are listed in Table 2.

Table 2

Mixture	Characteristic points	x_B	x_d	x_V	x_P	x_{df}
H$_2$–O$_2$	O	0.18	0.54	1	8.33	16.13
	B	—	—	0.18	0.33	0.543
H$_2$–air	O	0.186	0.56	1	6.67	13.16
	B	—	—	0.186	0.338	0.555
CH$_4$–O$_2$	O	0.114	0.54	1	12.5	25
	B	—	—	0.114	0.307	0.553
CH$_4$—air	O	0.163	0.55	1	7.69	14.46
	B	—	—	0.163	0.326	0.543
C$_2$H$_2$–O$_2$	O	0.115	0.54	1	14.3	22.18
	B	—	—	0.115	0.31	0.544
C$_2$H$_2$–air	O	0.16	0.55	1	8.33	16.58
	B	—	—	0.16	0.32	0.55
C$_2$H$_4$–O$_2$	O	0.107	0.54	1	14.3	21.06
	B	—	—	0.107	0.305	0.54
C$_2$H$_4$–air	O	0.159	0.55	1	8.33	15.6
	B	—	—	0.159	0.325	0.552

If B is chosen as the initial state of the combustible mixture, then the quadrant $P < P_B$, $V > V_B$ represents the domain of existence of deflagration processes for this state, and the Michelson–Rayleigh straight line from the point B also passing through the point O characterizes the maximum velocity of deflagration combustion. It should be noted that the states O and B are related by the mass and momentum conservation laws (see Fig. 2)

$$\rho_0 D = \rho_2(D - u_2) = \rho_B(D - u_B),$$

$$P_0 + \rho_0 D^2 = P_2 + \rho_2(D - u_2)^2 = P_B + \rho_B(D - u_B)^2,$$

which yields $(P_B - P_0)/(V_B - V_0) = -\rho_0^2 D_0^2 = \text{const}$ and admits the choice of any state (O or B) as the initial state. One more important conclusion can be drawn from Fig. 1: the flame velocity in the initial state O is noticeably smaller than the flame velocity at higher pressures and temperatures in the state B, which is clearly seen from the slope of the Michelson–Rayleigh straight lines 4 and 3 characterizing the combustion process in the states O and B (a greater slope from B is observed for line 3).

A specific feature of the state at the point B is the fact that there is a flow of the not yet reacted mixture behind the SW in this region; therefore, the flame front with respect to the laboratory coordinate system propagates over moving gas particles, i.e., its velocity is the sum of the flame velocity with respect to the particles and the flow velocity (this velocity is called the visible velocity of the flame). As the basic physical mechanisms of flame propagation are assumed to be heat conduction and diffusion, the combustion front should always have a subsonic velocity. Unfortunately, some researchers in recent publications incorrectly consider the visible velocity of the combustion front as the classical flame velocity and provide overestimated (including supersonic) values of this quantity, which is the substitution of the classical concepts.

For DW propagation over a quiescent mixture, we have

$$w_0 = D_d, w = D_d - u_d,$$

and the mass conservation law yields

$$u_d = D_d(1 - x_d^*) = D_d\left(1 - \frac{1 + \gamma M_d^2}{(\gamma + 1)M_d^2}\right)$$
$$= D_d\frac{M_d^2 - 1}{(\gamma + 1)M_d^2} \approx \frac{D_d}{\gamma + 1},$$

where u_d is the velocity of detonation products with respect to the motionless coordinate system. Simultaneously, the velocity of sound in the products is

$$c_d = D - u_d \approx [\gamma/(\gamma + 1)]D \approx \gamma u_d > u_d,$$

i.e., the flow of detonation products is subsonic.

However, the flow in the chemical spike (at the point B) at detonation (hypersonic) Mach numbers is supersonic with respect to the laboratory coordinate system:

$$u_N = D_d(1 - x_N^*) = D_d\Big(1 - \frac{(\gamma - 1)\mathrm{M}_d^2 + 2}{(\gamma + 1)\mathrm{M}_d^2}\Big)$$

$$= D_d\frac{2(\mathrm{M}_d^2 - 1)}{(\gamma + 1)\mathrm{M}_d^2} \approx \frac{2D_d}{\gamma + 1}.$$

Therefore, the starting chemical reaction decelerates the supersonic flow, and its velocity decreases (in a constant-section tube, the added heat accelerates the subsonic flow and decelerates the supersonic flow! [5]). In this case, the released heat of the chemical reaction increases the temperature of the mixture and the velocity of sound, i.e., the decreasing flow velocity and increasing velocity of sound come closer to each other. However, the transition from the supersonic to subsonic flow is only possible if the action changes, i.e., if heat supply is replaced with its removal. It should be emphasized that formally, with the Arrhenius exponential dependence of the chemical reaction rate on temperature, the reaction can be finalized only asymptotically, after an infinitely large time. The flow velocity has to approach the velocity of sound as close as possible, which is finalized by reaching the critical exhaustion velocity. In the Michelson–Chapman–Jouguet model, the sonic surface $w = c$ in the plane where the chemical reaction is finalized is postulated (it is called the Chapman–Jouguet plane). Within the framework of idealized models, the meaning of the Chapman–Jouguet plane is to ensure that weak perturbations do not pass to the wave front, which makes the region from the shock front to the sonic plane stay in a steady state. It is possible to add to this plane unsteady solutions in the form of acoustic rarefaction or compression waves, which do not affect the reaction zone.

As noted above, the Hugoniot curve at $Q = $ const is a hyperbola in the coordinate system (P, V) with the initial state point O. The coordinate system with the point B as the initial point is obtained by means of parallel transfer of the point O to the point B ($y' = y + a$, $x' = x + b$), which does not alter the character of the Hugoniot adiabat as a hyperbola.

Let us analyze the equation of the Hugoniot curve in the coordinate system (X, Y) with the initial state of the mixture at the point O in the case of passing to the coordinate system (X', Y') with the initial state at the point B. By analogy with the system (X, Y), we introduce the dimensionless variables $y' = P/P_B$ and $x' = V/V_B$. The Hugoniot curve (X, Y) is expressed via the new variables as

$$y = y'\frac{P_B}{P_0} = \frac{1 - \eta x'V_B/V_0 + 2\eta\gamma q}{x'V_B/V_0 - \eta};$$

from here, already in the system (X', Y'), we obtain

$$y' = \frac{1 - \eta x'V_B/V_0 + 2\eta\gamma q}{(x'V_B/V_0 - \eta)(P_B/P_0)}.$$

Here

$$\frac{P_B}{P_0} = \frac{2\gamma\mathrm{M}_0^2 - (\gamma - 1)}{(\gamma + 1)}, \quad \frac{V_B}{V_0} = \frac{(\gamma - 1)\mathrm{M}_0^2 + 2}{(\gamma + 1)\mathrm{M}_0^2},$$

while M_0 is the DW Mach number in the system (X, Y) with the point of the initial state of the mixture O. It is seen that the energy release adiabat in the coordinates (X', Y') remains a hyperbola, but it is deformed because of the emergence of constant factors P_B/P_0 and V_B/V_0. It should be specially emphasized that the tangency point of the Michelson–Rayleigh straight line with the energy release adiabat is not affected by passing from one system to the other. The tangency point characterizes the detonation process with respect to O and the deflagration process with respect to B. The coordinates of the tangency points are determined by means of the coupled solution of two equations: for the Michelson–Rayleigh straight line and for the energy release adiabat. The results of equilibrium computations of combustion and detonation parameters for several typical mixtures are listed in Table 3. Three first rows characterize the deflagration point F_O, detonation point D_O, and chemical spike point B for the initial state at the point O. Three next rows characterize similar parameters in the situation with the initial state being chosen at the point B (chemical spike of the DW).

It is seen that the specific energy release of the mixture Q_g in the case of detonation from the initial state at the point O and in the case of deflagration from the initial state at the point B is identical for different mixtures, which could be expected because compression in the bow front of the DW occurs under the assumption that the initial composition of the mixture remains unchanged, i.e., the shock wave transition is assumed to occur with no chemical reaction. The reaction begins and proceeds later. Because of the identical value of Q_g, the chemical composition of the products and the velocities of sound are also identical. These considerations confirm the presentation of detonation of the initial combustible mixture as deflagration (combustion) in a supersonic flow (columns for u_2 and c_2) in the chemical spike behind the bow shock front of the DW.

Let us analyze the entropy of the system from the viewpoint of choosing the initial state. Let us use the energy equation (energy release adiabat) in the form

$$U - (U_0 + Q) = (w_0^2 - w^2)/2 + P_0V_0 - PV$$

$$= (P + P_0)(V_0 - V)/2.$$

Table 3

Mixture	Characteristic points	D, m/s	u, m/s	c, m/s	Q_g, cal/s	u_2, m/s	c_2, m/s	M_d
H$_2$–O$_2$	F_O	84	−1258	1342	1891	—	—	—
	D_O	2837	1294	1543	1580	—	—	5.283
	B	—	—	—	—	2328	1268	—
	F_B	508	−1034	1542	1580	—	—	—
	D_B	2748	1045	1703	1242	—	—	2.168
	B	—	—	—	—	1891	1602	—
H$_2$–air	F_O	71	−872	943	777	—	—	—
	D_O	1969	878	1091	673	—	—	4.819
	B	—	—	—	—	1602	896	—
	F_B	366	−726	1091	673	—	—	—
	D_B	1941	729	1212	537	—	—	2.167
	B	—	—	—	—	1331	1139	—
CH$_4$–O$_2$	F_O	45	−1065	1110	1348	—	—	—
	D_O	2390	1101	1289	1141	—	—	6.731
	B	—	—	—	—	2119	826	—
	F_B	271	−1018	1289	1141	—	—	—
	D_B	2492	1032	1460	888	—	—	3.016
	B	—	—	—	—	2061	1065	—
CH$_4$–air	F_O	53	−800	860	643	—	—	—
	D_O	1803	805	998	559	—	—	5.089
	B	—	—	—	—	1509	759	—
	F_B	294	−704	998	559	—	—	—
	D_B	1827	707	1119	440	—	—	2.406
	B	—	—	—	—	1351	970	—
C$_2$H$_2$–O$_2$	F_O	40	−1063	1103	1200	—	—	—
	D_O	2424	1108	1316	973	—	—	7.342
	B	—	—	—	—	2146	851	—
	F_B	278	−1038	1316	973	—	—	—
	D_B	2590	1056	1534	691	—	—	3.043
	B	—	—	—	—	2107	1160	—

Table 3 (continued)

Mixture	Characteristic points	D, m/s	u, m/s	c, m/s	Q_g, cal/s	u_2, m/s	c_2, m/s	M_d
C$_2$H$_2$–air	F_O	54	−828	883	722	—	—	—
	D_O	1866	840	1026	588	—	—	5.378
	B	—	—	—	—	1566	784	—
	F_B	300	−726	1026	588	—	—	—
	D_B	1890	731	1159	443	—	—	2.412
	B	—	—	—	—	1387	1019	—
C$_2$H$_4$–O$_2$	F_O	39	−1051	1091	1255	—	—	—
	D_O	2374	1092	1282	1048	—	—	7.236
	B	—	—	—	—	2120	798	—
	F_B	254	−1028	1282	1047	—	—	—
	D_B	2517	1046	1472	788	—	—	3.154
	B	—	—	—	—	2100	1056	—
C$_2$H$_4$–air	F_O	56	−811	867	678	—	—	—
	D_O	1824	819	1005	570	—	—	5.260
	B	—	—	—	—	1533	761	—
	F_B	291	−714	1005	570	—	—	—
	D_B	1849	718	1131	436	—	—	2.431
	B	—	—	—	—	1370	980	—

In the differential form, with due allowance for the first law of thermodynamics, this equation looks as follows:

$$dU = (V_0 - V)/2 \cdot dP - (P + P_0)/2 \cdot dV$$
$$= T \cdot dS - P \cdot dV,$$

whence it follows that

$$T \cdot dS = (P - P_0)/2 \cdot dV - (V - V_0)/2 \cdot dP.$$

The equation of the Michelson–Rayleigh straight line is

$$(P - P_0)(V - V_0) = -\rho_0^2 w^2 = \text{const},$$

therefore, at the tangency points of the Michelson–Rayleigh straight lines and the energy release adiabat, the last relation yields $T \cdot dS = 0$, and the entropy of the system reaches extreme values (both at the detonation and deflagration points). The values of entropy at the tangency points characterize its individual isentropes (curves $S = $ const or $PV^\gamma = $ const) for detonation and deflagration; moreover, by virtue of the extreme property, these isentropes are tangent lines both to the Michelson–Rayleigh straight lines and to the Hugoniot curve. The character of the extreme point of entropy is determined by the second derivative of the above-presented expression for the Hugoniot curve

$$2T \frac{dS}{dV} = (P - P_0) - (V - V_0)\frac{dP}{dV}.$$

We have

$$2T \frac{d^2 S}{dV^2} = -(V - V_0)\frac{d^2 P}{dV^2}.$$

As the Hugoniot adiabat is a hyperbola, then $\frac{d^2 P}{dV^2} > 0$; therefore, $\frac{d^2 S}{dV^2} > 0$ for $V < V_0$ (detonation point with the entropy minimum if the isentrope touches the Hugoniot curve from below) and $\frac{d^2 S}{dV^2} < 0$ for $V > V_0$ (deflagration point with the entropy maximum if the isentrope touches the Hugoniot curve from above). Thus, if the state of the system changes from the initial state at the point O to the state in the chemical spike B of the detonation wave, it is not only the Hugoniot curve equation that changes, but also the character of the extreme point of the isentrope (from the minimum to the maximum) and, correspondingly, the mutual locations of the Hugoniot adiabat and isentrope. In view of the preliminary change from the state O to B, the subsequent chemical reaction is finalized identically: the entropy of the system tends to the maximum value, fully in line with the second law of thermodynamics. This result can be considered as a proof that detonation can be really considered as combustion in a flow of a combustible mixture, and the detonation mixture itself can be considered as a system subjected to two-fold irre-

versible conversion, first, owing to the action of the bow shock front, and then owing to the chemical reaction of mixture combustion.

CONCLUSIONS

It is shown that the minimum increase in entropy of the combustible mixture in the case of detonation as compared to its maximum increase in the case of deflagration predicted by the classical idealized models is associated only with the factor of the entropy increase in the irreversible chemical reaction of the mixture, while the entropy increase due to an irreversible transition of the initial mixture to the Neumann spike state behind the bow shock wave of the detonation front was ignored. The allowance for the two-stage increase in entropy in the case of detonation (irreversible transition under shock wave compression of the mixture with subsequent irreversible chemical transformation of the initial mixture to detonation products) makes it possible to eliminate the contradiction concerning the character of the change in entropy during an irreversible detonation process, which is predicted by the classical models.

The allowance for the intermediate transition of the mixture from the initial state to the state in the Neumann spike of the detonation wave proves Shchelkin's prediction of the possibility of considering detonation as combustion of a combustible mixture in a supersonic flow.

REFERENCES

1. *Physics of Explosion*, Ed. by L. P. Orlenko (Fizmatlit, Moscow, 2002) [in Russian].
2. K. I. Shchelkin and Ya. K. Troshin, *Gas-Dynamics of Combustion* (Izd. Akad. Nauk SSSR, Moscow, 1963) [in Russian].
3. F. Bartlma, *Gasdynamik der Verbrennung* (Springer-Verlag, Wien, 1975).
4. N. M. Bazhin, V. A. Ivanchenko, and V. N. Parmon, *Thermodynamics for Chemists* (Khmimiya–KolosS, Moscow, 2004) [in Russian].
5. K. P. Stanyukovich, *Unsteady Motions of Continuous Media* (Nauka–GRFMLit, Moscow, 1971) [in Russian].