

Resonance of Oscillations between the Reaction Products and Initial Mixture As a Reason for the Deflagration-to-Detonation Transition

A. A. Vasil'ev^{a,*}

UDC 544.452+544.454

Published in *Fizika Goreniya i Vzryva*, Vol. 58, No. 3, pp. 71–79, May–June, 2022.
Original article submitted December 12, 2021; revision submitted January 12, 2022; accepted for publication January 12, 2022.

Abstract: Qualitative transformation of a low-velocity laminar flow to a turbulent state (owing to natural or artificial instability) and formation of compression waves passing ahead have been studied in much detail. A disputable issue is the nature of the emergence of a reaction pocket in the region between the bow compression wave and the flame front moving at a certain distance behind this wave, as well as the dynamics of interaction of this pocket with the main structural elements. It is the type of this pocket (slow or explosive combustion) that defines its subsequent interaction with the compression wave front: shockless or shock-induced expansion capable of forming a detonation wave. As a method of transforming the reaction pocket to an explosion pocket, its amplification owing to the resonance of streamwise acoustic oscillations of hot reaction products with the initial combustible mixture induced by flame propagation is discussed. It is the resonance with its multiple enhancement of the amplitude of gas-dynamic parameters that can effectively initiate the deflagration-to-detonation transition. Various stages of this transition are discussed; the corresponding estimates are made and are found to be consistent with experiments.

Keywords: deflagration-to-detonation transition, subsonic and supersonic flows, reacting media, resonance of oscillations.

DOI: 10.1134/S0010508222030078

INTRODUCTION

The most important problem of combustion and explosion science is the deflagration-to-detonation transition (DDT), which is a system of unsteady and quasi-steady regimes in combustible mixtures. This system includes excitation of slow chemical reactions, flame formation, development of its instability, acceleration of the flame front to transonic velocities, transition to a supersonic regime with formation of the bow shock wave (SW), emergence of a new pocket of the chemical reaction in the region of the mixture compressed and heated by the SW, dynamics of subsequent evolution of this pocket, and character of interaction of the

pocket with the bow shock wave, including its amplification and subsequent acceleration to detonation velocities.

Modeling of the DDT process is impossible without a clear idea about the DDT dynamics and without knowing its governing parameters at each stage with due allowance for the space and time parameters of the combustible mixture. This is particularly important from the viewpoint of safety in emergency situations, where it is necessary to clearly understand possible scenarios of the emergence and evolution of the combustion pocket under real conditions for estimating the consequences of unauthorized ignition or explosion in order to ensure the maximum safety of people and equipment and to minimize the action of hot products on them. In this paper, an attempt is made to attract attention to the problem of taking into account the resonance phenomena in DDT modeling.

^aLavrentyev Institute of Hydrodynamics, Siberian Branch, Russian Academy of Sciences, Novosibirsk, 630090 Russia;
*gasdet@hydro.nsc.ru.
Novosibirsk State University, Novosibirsk, 630090 Russia.

INITIATION OF THE CHEMICAL REACTION IN A COMBUSTIBLE MIXTURE

It is well known that mixing of a gaseous fuel and oxidizer and formation of a combustible mixture do not lead to an immediate chemical reaction between them, and the mixture can remain in such a state for a long time [1–4]. This metastability of the mixture is associated with the existence of a potential barriers (activation energy E_a), which means that particles can give rise to the chemical reaction after overcoming this barrier. Within the framework of the ideal gas model, the chemical reaction between the fuel and oxidizer is initiated by particle collisions and starts under the condition that this potential barrier is overcome by a “necessary” number of active particles. The Maxwell distribution functions of particles in terms of their velocities are defined by the formulas $f(v) = (m/2\pi kT)^{3/2} \exp(-mv^2/2kT)$ and $F(v) = 4\pi v^2(m/2\pi kT)^{3/2} \exp(-mv^2/2kT)$, where m is the mass of the particles, and k is the Boltzmann constant. The condition of normalization for the absolute values of velocity is $\int_0^{\infty} F(v)dv = 1$ [5, 6]. The upper un-

bounded limit of the integral is a mathematical abstraction because real particle velocities do not have such values. Nevertheless, such an abstraction allows one to estimate the number of particles with this velocity by the formula $dN = 4\pi N v^2 (m/2\pi kT)^{3/2} \exp(-mv^2/2kT)$ and also to estimate the number of particles with energies is higher than the activation energy: $mv^2/2 > E_a$.

In accordance with the Maxwell functions, there are always active particles present in the flow. To explain metastability of the mixture under normal conditions, we have to assume that the reaction in a medium with a small number of active particles decays (or proceeds extremely slowly) rather than develops. For the reaction to proceed, the number of active particles should be increased to a certain minimum necessary value $N = N^*$, which is not known in advance. This can be done with the use of an external initiator. Then the energy E_{ign} introduced into the mixture by this initiator can be estimated as $E_{\text{ign}} = N^* E_a$. At $E \geq E_{\text{ign}}$, excitation of the chemical reaction should be initiated in the zone of active particles, which then would be able to extend to the entire volume of the combustible mixture not only in the slow regime, but also in the accelerating subsonic regime.

Chemical kinetics defines the reaction rate W as a function proportional to the concentrations of the reacting substances $W(T, c) = \frac{dc}{dt} = k(T)F(c) > 0$,

$F(c) = c_A^{n_A} c_B^{n_B} \dots c_G^{n_G} \dots$ [5]. The temperature dependence of the reaction rate constant $k(T)$ is known to obey the empirical Van't Hoff rule: as the temperature increases by each ten degrees, the constant $k(T)$ increases approximately by a factor of 2–4: $\delta = k_{T+10}/k_T = 2-4$ or $W(T_2)/W(T_1) = \delta^{(T_2-T_1)/10}$. This empirical rule, which allows one to estimate the influence of temperature on the chemical reaction rate in the first approximation, was experimentally verified in a moderate temperature interval (usually from 0 to 100°C). Later on, Arrhenius derived the famous limit $\lim_{n \rightarrow \infty} (1 + 1/n)^n = e$ for $k(T)$: $k(T) = k_0 \exp(-E_a/RT)$ (the exponential function $e = \exp$ is not changed by differentiation and integration!). The term “constant” is not very good for $k(T)$ because $k_0 = \varphi(T)$!

The qualitative behavior of the reaction rate as a function of timer is shown in Fig. 1a: slow increase at the initial stage (during the induction period τ_{ind}) with gradual enhancement and reaching the maximum rate, followed by gradual reduction of the reaction rate caused by consumption of the reacting components. This reaction rate profile corresponds to the energy release in the mixture (Fig. 1b) as an integral of the reaction rate multiplied by the specific energy release in the mixture.

INITIATORS FOR OVERCOMING THE ACTIVATION BARRIER

The barrier can be overcome with the use of an external source. A source traditionally used for excitation of combustion waves in a reacting mixture is a thermal igniter (hot body, heated wire, open fire, etc.). The initiator most often used in engineering devices is an electric spark.

It was found in experimental on studying the temperature dependence $W(T)$ that the mixture ignition process is characterized by two temperatures: flash temperature (the mixture bursts when a heat source is set close to the mixture, but ceases to burn when the source is moved away from the mixture) and ignition temperature (the mixture bursts when a heat source is set close to the mixture and continues to burn when the source is removed from the mixture). The values of the flash temperature are significantly scattered, and this parameter is not widely used [7]. The ignition temperature T_{ign} is an important parameter: at $T < T_{\text{ign}}$, the mixture is able to burn only near the igniter, and combustion decays with distance from the heat source; the condition $T > T_{\text{ign}}$ has to ensure combustion wave propagation over the entire volume of the mixture.

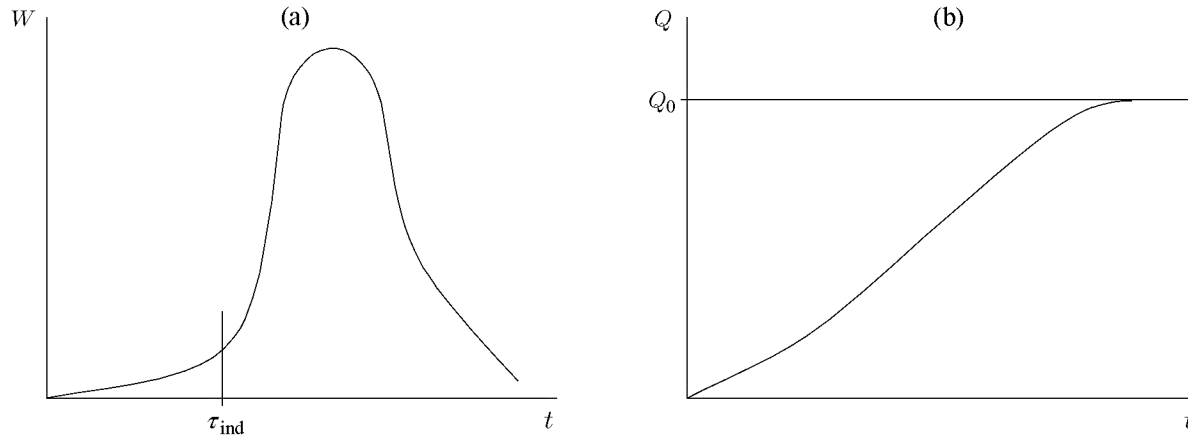


Fig. 1. Chemical reaction rate W (a) and energy release Q (b) versus time.

The initial stage of ignition of the mixture is determined by the external initiator, and the energy release from the mixture at this stage is negligibly small. As the combustion front propagates over the mixture, the role of the initiator decreases, and the energy for supporting the combustion wave has to be extracted from the mixture itself owing to the thermal effect of the chemical reaction Q . It should be noted that the ignition temperature T_{ign} is also characterized by noticeable scatter caused by weak repetitivity of initiating pulses in different experiments and spontaneous dynamics of the energy release in the mixture. The flash and ignition temperature are usually used to describe slowly proceeding chemical reactions.

In the case of adiabatic or shock wave compression, the mixture can ignite without the external source at the self-ignition temperature $T_{\text{self-ign}}$. In combustion, the reactions proceed sufficiently rapidly; therefore, the self-ignition temperature, which is more clearly determined, is used in practice most often to describe the process of excitation of propagating flames. The effect of combustion initiation in combustible mixtures usually has a “threshold” character (go–no go) for any initiator. Initiation can be compared with the relay exchange of the energy supply from the external source to the energy release from the combustible mixture.

Detonation initiators can be a powerful electric or laser spark (breakdown), exploding wire, high-velocity flow of hot and active particles, explosive charge, etc. All initiators have individual space and time characteristics of energy input to the mixture. They are divided into ideal and non-ideal [8] sources depending on the relationship of the space and time parameters of the initiator and combustible mixture. For detonation to be initiated, the external initiator has to generate an SW behind which the initially quiescent mixture is trans-

formed to a gas flow, and the conditions of ignition of the moving mixture are noticeably more complicated. The governing parameters here are the self-ignition temperature $T_{\text{self-ign}}$ and the ignition delay of the reacting mixture. The initiator has to sustain this temperature for a time period sufficient for the chemical reaction development up to a stage at which further propagation of the detonation wave can be supported by the energy release in the mixture Q . Excitation of detonation propagating in the self-sustained regime over the entire volume of the combustible mixture also has a “threshold” character (no–no go) for any initiator.

TYPICAL FLAMES AND VELOCITIES OF THEIR PROPAGATION

The modern classification of the processes observed in the combustible mixture looks as follows.

1. Combustion:

- laminar combustion (velocities of several tens of centimeters per second);
- turbulent combustion (velocities up to several tens of meters per second);
- accelerating flames, i.e., an increase in the amplitude of unstable harmonics in addition to flame transfer by the flow (up to transonic velocities).

2. Transient regimes of unsteady propagation with SW formation and possible DDT (supersonic velocities).

3. Detonation (velocities of several kilometers per second, e.g., $D_0 = 2.840$ km/s in the $2\text{H}_2 + \text{O}_2$ mixture).

In idealized models of flame propagation with a flat front, the basic characteristic is assumed to be the normal flame velocity S_u [1, 3, 4]. In motionless systems, it is derived with the use of the Fourier and Fick laws on proportionality of the heat and mass flux den-

sities (per unit time through a unit area) to the gradients of the corresponding parameters $q_T = -\lambda \frac{\partial T}{\partial x_n}$ and $q_C = -\hat{D} \frac{\partial C}{\partial x_n}$, where λ [J/(m·s·K)] is the thermal conductivity, \hat{D} [m²/s] is the diffusion coefficient, T is the temperature, and C is the concentration; the subscript n corresponds to the normal to the flame front element under consideration [6]. In the mixture moving with a velocity v , the transport equations are transformed to $q_T = -\lambda \text{grad}T + \rho c_p TV$ and $j_C = -\hat{D} \text{grad}C + CV$, where ρ is the density, c_p is the heat capacity at constant pressure, and V is the volume. If there are chemical reactions in a motionless system, then these equations in the case with the gradients of the temperature T and concentration C look as follows:

$$\frac{\partial C}{\partial t} = \text{div}(\hat{D} \text{grad}C) + q', \quad c_p \rho \frac{\partial T}{\partial t} = \text{div}(\lambda \text{grad}T) + q''.$$

Here q' [mol/s] is the reaction rate, and q'' [J/(m³·s)] is the power density of the energy release in the mixture.

The minimum velocity of propagation determined by the thermal conductivity and diffusion is typical for the laminar flame (of the order of several centimeters per second). The formula $\langle \Delta x^2 \rangle = 2\hat{D}t$ was derived for the mean square of the particle displacement due to diffusion, though the mean particle displacement is assumed to be equal to zero: $\langle \Delta x \rangle = 0$. At the same time, the Brownian motion of particles is well known, where the particle “moves away” from the initial point with time. Then, the mean displacement of the particle can be determined via its mean square of its displacement: $|\langle x \rangle| = \sqrt{\langle \Delta x^2 \rangle} \approx \sqrt{2\hat{D}\tau} \cong \langle S_{\text{diff}} \rangle \tau$. The latter equality follows from the classical definition according to which the particle moves per unit time interval [1 s] to a distance numerically equal to its mean velocity. This fact allows one to estimate the diffusion rate $S_{\text{diff}} = \sqrt{2\hat{D}/[1 \text{ s}]}$ (the dimension of \hat{D} being cm²/s, the dimension of S_{diff} is cm/s). For example, for oxygen molecules under standard conditions, we have $\hat{D} \approx 0.2$ cm²/s, which yields $S_{\text{diff}} \approx 0.6$ cm/s [9]. The diffusion rate is very small as compared to any other velocity used in molecular physics: $v \equiv v_{\text{max}} = \sqrt{2kT/m} = \sqrt{2RT/\mu}$, $\langle v \rangle = \sqrt{8kT/\pi m} = \sqrt{8RT/\pi\mu}$, $\langle v^2 \rangle = \sqrt{3kT/m} = \sqrt{3RT/\mu}$, and $c = \sqrt{\gamma RT/\mu}$, where μ is the mole mass, and c is the velocity of sound.

Landau [10] theoretically predicted the absolute instability of the flat flame front because small perturbations of parameters (even in the linear approximation) were enhanced, and the flame front lost its flat character, first of all, because of the governing effect of temperature on the chemical reaction rates. Flames with an unstable structure of the front are called turbulent

flames (by analogy with hydrodynamic flows of continuous media). In fact, laminar combustion is realized in rare cases; most often, combustion proceeds in the turbulent mode. The main reason is the existence of convective fluxes of hot reaction products whose directions rarely coincide with the flame propagation direction. A key role in the transformation of the laminar to turbulent flame belongs to the fact that the characteristics of heat transfer and diffusion of active particles in a turbulent flow are noticeably greater than those in the laminar flame. These characteristics also assist in the development of instability and turbulization of the reaction region.

If the source terms q' and q'' are chosen to be proportional to the Arrhenius dependence of the reaction rate $W(T, c)$, then the equations for heat propagation and diffusion can be made identical at the Lewis number $Le = \hat{D}/\zeta = \hat{D}\rho c_p/\lambda \approx 1$ (ζ [m²/s] is the thermal diffusivity) and certain boundary and initial conditions. The method of solving these equations and the assumptions used were described in sufficient detail in many reference books (e.g., [3, 4]).

Using the heat conduction equations for plane symmetry $\frac{\partial T}{\partial t} = \zeta^2 \frac{\partial^2 T}{\partial x^2}$, Mikhelson [1] derived the temperature distribution ahead of the flame front for a steady flame: $T = T_0 + A \exp(-S_u x/\zeta)$; then the characteristic scale of the heating region (a change by a factor of e) is $\delta = \zeta/S_u$. For example, for a stoichiometric CH₄-air mixture, $S_u = 40$ cm/s and $\zeta \approx 0.22$ cm²/s; then, $\delta \approx 6 \cdot 10^{-3}$ cm. For a 2H₂ + O₂ mixture with the maximum velocity $S_u = 1000$ cm/s, we have $\delta \approx 4 \cdot 10^{-4}$ cm. The corresponding time of particle residence in the heating region is $t_\delta = \delta/S_u \approx 1.4 \cdot 10^{-4}$ s in the methane-based mixture and $t_\delta \approx 4 \cdot 10^{-7}$ s in the hydrogen-based mixture.

Using the dimensional theory and the heat conduction equation $\frac{\partial T}{\partial t} = \zeta \Delta T$, one can find the functional relationship of the characteristic spatial scale of the reaction region δ with the thermal diffusivity of the medium ζ and characteristic time of mixture burning τ_r ($1/\tau_r \approx \zeta/\delta^2$) from which the normal flame velocity is estimated as $u_n \approx \delta/\tau_r \approx \sqrt{\zeta/\tau_r} \ll c_0$. The velocity of laminar flame propagation $S_{\text{lamin}} = \sqrt{\zeta/\tau_r}$ is an eigenvalue, where $\tau_r = [A \exp(-E/RT)]^{-1}$ is the characteristic reaction time. The dependence of the laminar flame velocity on pressure and temperature is described by the approximate formula $S_{\text{lamin}} \approx p^{n/2-1} \exp(-E/RT_f)$ [7].

In the classical thermodynamics and molecular physics (see, e.g., [6]) within the framework of the ideal gas model, the following relations were established between the thermal diffusivity $\zeta = \lambda/\rho c_p$, kine-

matic viscosity $\nu = \mu/\rho$, and diffusion coefficient \hat{D} : $\zeta = \hat{D} = \nu = \text{const} \cdot \langle u \rangle$, where $\langle u \rangle$ is the velocity of thermal motion of molecules. It should be specially emphasized that the normal flame velocity is always much smaller than the velocity of sound in the initial mixture: $u_n \ll c_0$; therefore, it follows from the equality $\zeta = \hat{D} = \nu$ that neither turbulence, nor diffusion, nor heat conduction can ensure acceleration of the laminar combustion wave to sonic values; moreover, these phenomena even cannot transform the process to supersonic velocities that are extremely important in the DDT case!

This conclusion can be additionally confirmed by the following estimates. Investigations of flame propagation in tubes (horizontal and vertical, with closed or open end faces, including situations with one end face) showed that the laminar flame velocity (marked by the subscript L) with respect to the unburned (u) mixture can be estimated from the condition that the ratio of the volume velocity of the flow vS [m^3/s] to the flame front area S_{flame} [m^2] is constant $S_L \equiv S_u = v \cdot S / S_{\text{flame}}$; here S is the cross-sectional area of the tube, and v is the flow velocity [2, 7]. With respect to the burned (b) gas, the flame velocity is $S_b = S_L \cdot \rho_u / \rho_b > S_L$. Sometimes the turbulent flame velocity is approximated by the expression $S_{\text{turb}} = S_L \cdot \sqrt{\text{Re}} = S_L \cdot \sqrt{vd/\nu}$, where ν [m^2/s] is the kinematic viscosity, and d [m] is the characteristic scale of the flow.

For most hydrocarbons, the numerical values of the maximum flame velocity S_u for gas mixtures are 40–60 cm/s; slightly higher values were obtained for ethylene (80 cm/s) and acetylene (160 cm/s). A record-holder is hydrogen whose flame velocity is greater almost by an order of magnitude than those of hydrocarbons: 3–10 m/s. The velocity $S_u \approx 10$ m/s for a stoichiometric hydrogen–oxygen mixture corresponds to the Mach number $M_n = S_u/c_0 \approx 10/540 \approx 1.8 \cdot 10^{-2}$. For most hydrocarbon mixtures, the Mach number is smaller by an order of magnitude: $M_n = S_u/c_0 \approx 0.5/300 \approx 1.7 \cdot 10^{-3}$. For such a low Mach number, the slope of the Mikhelson–Rayleigh straight line (analog of the laws of conservation of mass and momentum of the mixture in passing through the flame front) is almost invisible, and the final of combustion products is little different from the state obtained in combustion at $p = \text{const}$. This fact allows one to use the well-developed and self-consistent system of thermodynamic data of the detonation theory for the analysis.

Let us estimate the increase in the area of the turbulent flame front, as compared to the plane flame area, needed to reach some characteristic velocities, for example, for mixture of a typical hydrocarbon with oxygen: $C_xH_y-O_2$. Using the law of areas for

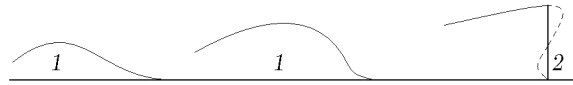


Fig. 2. Qualitative pattern of sharpening of the bow shock wave and emergence of a nonunique fold at the wave front (dashed curve): (1) disturbed region; (2) replacement of the fold by a discontinuity.

laminar–turbulent flames $S_t = S_n \cdot \Omega_t/\Omega_n$, we find that, for flame acceleration from the laminar velocity $S_n = 0.4$ m/s to the deflagration velocity $S_{\text{def}} = 60$ m/s, the flame front surface should be increased by a factor of $\Omega_t/\Omega_n = 60/0.4 = 150$. For the flame to be accelerated to the velocity of sound $c_0 = 320$ m/s, the area should be increased by a much greater factor $\Omega_t/\Omega_n = 320/0.4 = 800$, and flame acceleration to the detonation velocity $D_0 = 2400$ m/s requires the area to be increased by a factor $\Omega_t/\Omega_n = 2400/0.4 = 6000$! No information about obtaining such values owing to self-turbulization of the flame front was found in scientific literature, though the positive effect in flame acceleration owing to artificial turbulization of the flow is well known (e.g., the famous Shchelkin’s spiral).

A similar increase in the front area can be reached in an expanding cylindrical or spherical flame, but no reliable experimental evidence was found on reaching at least sonic velocities due to self-turbulization of the front. Self-turbulization of the front owing to instability development favors an increase in velocity and a transition to turbulent combustion with velocities at the level often meters per second. The front of an accelerating (but low-velocity) flame generated compression waves passing ahead. Each next wave catching up the previous wave increases the slope of the bow shock wave (see Fig. 2). Beginning from some time instant, the bow shock wave acquires a nonunique shape where the wave top overtakes the wave foot (so-called wave “breakdown,” see the dashed curve in the right part of Fig. 2). For simplification, mathematicians replace this “broken” wave by a discontinuity surface (curve 2).

Figure 3 shows an idealized pattern of a one-dimensional flow with accelerated motion of a piston (curve 02), where the C+ characteristics emanating from the piston form a fan of converging straight lines. In some publications, this point of intersection of characteristics is even interpreted as a point of SW emergence(?). No attention is paid to the necessary property for the SW of its supersonic propagation with respect to the quiescent gas. A vivid example of a “broken” wave is a water wave near the shore (Fig. 4): one can clearly see the wave breakdown, but nobody even detected any supersonic phenomena (even in a storm)!

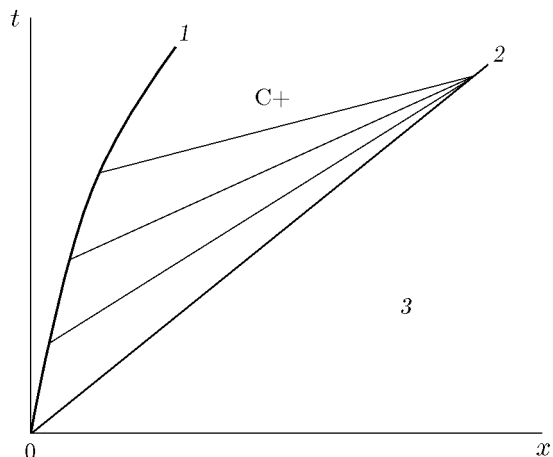


Fig. 3. Mathematical idealization of the emergence of the discontinuity 2 as an intersection of C+ characteristics emanating due to accelerated motion of the piston (its trajectory is curve 01) into domain 3 of the hot mixture.

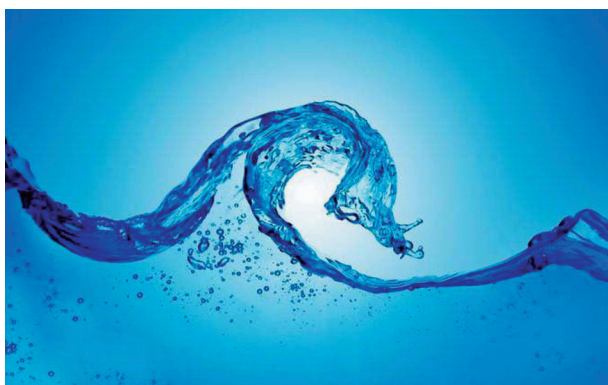


Fig. 4. Photograph of the water wave and its “break-down” (nothing like supersonic propagation).

WHICH PARAMETER OF THE MIXTURE DETERMINES THE DEFLAGRATION-TO-DETONATION TRANSITION?

As was noted above, neither turbulence, nor diffusion, not heat conduction can accelerate the laminar combustion wave to sonic velocities, leaving aside supersonics. Let us consider other parameters. Thus, the idealized theory implies that the combustion and detonation regimes are described by the Hugoniot curve with the condition $Q = \text{const}$ (“frozen” adiabat). This means that the final compositions of reaction products and temperatures are identical in combustion and detonation regimes. As the combustion and detonation velocities differ by several orders of magnitude, it can be concluded that the specific heat release Q and the

temperature of the products cannot serve as governing parameters for the DDT. The situation is not improved by eliminating the condition $Q = \text{const}$ and replacing it by the condition of chemical equilibrium of the products $Q = Q(p, T) \neq \text{const}$ (“equilibrium” adiabat, which is less steep than the “frozen” adiabat).

Generation of acoustic compression waves passing ahead by the flame does not create a flux of particles in the direction of flame front propagation along the tube. This role cannot be provided by the classical heat conduction and diffusion. Particle motion can be triggered by a comparatively powerful external initiator (the simplest example is the car spark plug). After its activation, the initiator can not only ignite the mixture, but also set the combustion products being formed into motion in the region adjacent to the initiator (radially diverging motion in the case of point initiation or motion directed along the tube in the case of initiation at the closed end face of the tube). These moving combustion products expand like a “piston” and generate an SW running away from the initiator. If the parameters behind such a wave can ignite new portions of the combustible mixture, then the process will propagate further.

If the external initiator power is low (e.g., glowing filament), then the mixture can be set into motion by thermal-diffusion convection. The essence of thermal-diffusion convection is the fact that hot combustion products in the gravity field try to move upward and are replaced by molecules of the initial cold mixture, i.e., in addition to random motion in the system, there arises directed motion (including vortex motion). It is the motion and its basic characteristic, mass velocity of the flow, that can be considered as the governing parameters of the DDT. An additional argument is the known fact that the translational degrees of freedom of particles are excited most rapidly.

ENERGY RELEASE IN THE FLOWS

It should be specially emphasized that the flows formed after ignition are obviously subsonic; therefore, in accordance with gas-dynamic laws [11], the chemical energy released during combustion accelerates the subsonic flow in a constant-area tube, thus, accelerating the “piston” action on the fresh mixture. Simultaneously with the increase in the mass velocity of the subsonic flow, the temperature also increases due to the heat released in the reaction, as well as the velocity of sound. The values of the mass velocity and the velocity of sound come closer to each other, and the flow turns to a transonic flow. However, again according to gas-

Table

Mixture (stoich.)	c_1 , m/s	c_3 , m/s	c_1/c_3
H ₂ -O ₂	537	1342	0.4
H ₂ -air	409	943	0.43
CH ₄ -O ₂	355	1110	0.32
CH ₄ -air	354	860	0.41
C ₂ H ₄ -O ₂	328	1091	0.3
C ₂ H ₄ -air	347	867	0.4
C ₂ H ₂ -O ₂	330	1103	0.3
C ₂ H ₂ -air	347	883	0.39

dynamic laws, a transonic flow in a constant-area tube cannot be transformed to a supersonic regime: (a) either without changing the tube cross section (e.g., with the Laval nozzle); (b) in the case of an unchanged tube cross section) owing to replacement of energy input by energy output (a change in the energy exchange sign). The latter is particularly important for the DDT, where the energy released due to mixture burning is effective at the stage of acceleration of the low-velocity of the flow to a transonic velocity, but it is almost ineffective at the next stages because the energy is still released, but it cannot transform a subsonic flow to a supersonic velocity.

An additional illustration for the reasoning above is the plot of the relationship between the mass velocity of the flow u (solid curves) and the velocity of sound c (dotted curves) as functions of the SW Mach number in Fig. 5 (stoichiometric mixtures of hydrogen and air; $u = 0$ and $c = c_0$ at $M = 1$). It is seen that the transonic regime behind the SW $u \approx c$ (vertical dashed curve) is reached at a moderate Mach number $M \approx 2$. At $M > 2$, the flow behind the SW becomes supersonic; then the energy, which continues to be released due to mixture combustion, decelerates this supersonic flow. Therefore, there are no reasons for the DDT to occur from $M \approx 2$ to the detonation regime with $M \approx 5$. It should be also noted (see Fig. 5) that the subsonic laminar or turbulent velocity of the combustion front with respect to motionless particles (classical) in the transonic region is added to the flow velocity, which reaches several hundreds meters per second. This total velocity with respect to the motionless tube has a physical meaning of the visible rather than classical velocity of the flame front. The visible velocity as a nonphysical variable can even exceed the velocity of sound in the initial mixture. In addition, the Mach number of the visible DDT of the flame front detected experimentally in the DDT case is close to the value provided above: $M \approx 2$.

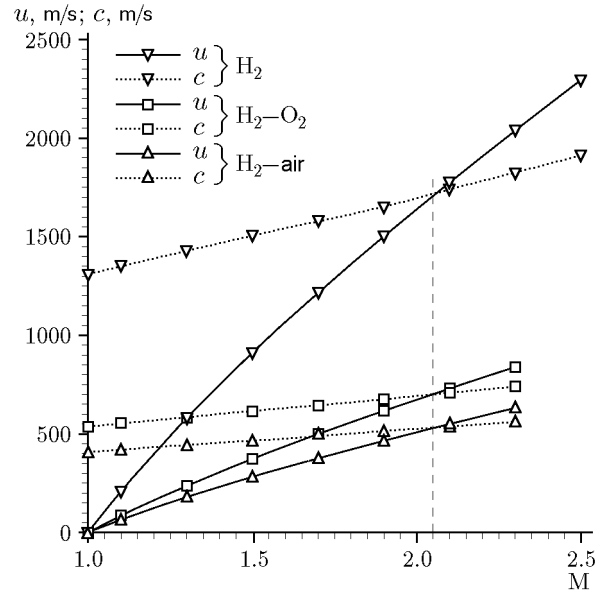


Fig. 5. Mass velocity and velocity of sound behind the SW front propagating in pure hydrogen in stoichiometric hydrogen-oxygen and hydrogen-air mixtures: at $M = 2.05$, the flow behind the SW transforms from the subsonic to supersonic regime.

The discussion above is insufficient to answer the question how it is possible to form a powerful shock wave and accelerate the flow to a supersonic velocity by using subsonic processes of heat conduction and diffusion, as well as acoustic perturbations generated by the “piston.” Experimenters use various artificial initiators of the DDT (Shchelkin’s spiral, grids, disks with orifices, rod structures, and channel contouring). Theoreticians try to “improve” the turbulence models.

ON ACOUSTIC PROPERTIES OF THE COMBUSTIBLE MIXTURE AND ITS PRODUCTS. RESONANCE

One more important aspect is the role of acoustic vibrations of combustion products. The importance of this issue is well known for specialists by an example of the nature of spin detonation in a circular tube, where the rotational velocity of the transverse wave exactly coincided with the velocity of the principal mode of axial acoustic vibrations of detonation products [7].

Let us consider the simplest scheme of flame propagation along the tube of length L_0 with a constant cross section (diameter d) and with open ends (to avoid reflections). Let the flame be transferred from one end face of the tube to the other in the mixture flow (velocity u), propagating with respect to the moving particles of the

mixture with a certain turbulent velocity S_t : (1) initial mixture; (2) flame front; (3) combustion products. In the initial mixture, the wave length of radial vibrations λ_{1n} is determined by the tube diameter $\lambda_{1n} = 2d/n$, and the frequency is $\nu_{1n} = c_{10}/\lambda_{1n} = nc_{1n}/2d$. In the combustion products, we have $\lambda_{3n} = \lambda_{1n}$ and $\nu_{3n} = c_{30}/\lambda_{3n}$; then, $\nu_{3n}/\nu_{1n} = c_{30}/c_{10}$. Among the axial vibrations, the most important mode is that with $\lambda_\varphi = \pi d$ for which $\nu_{3\varphi}/\nu_{1\varphi} = c_{30}/c_{10}$. In view of the low probability of the integer ratio of the velocities of sound in the combustion products and initial mixture (the data for some mixtures are listed in the table), it can be concluded that the resonance is possible in the regions under study in neither radial nor axial vibrations.

At the same time, there are streamwise oscillations of the gas in the system consisting of the initial mixture and reaction products with a moving interface (at the combustion front). Let us indicate the lengths of the domains of the burned and initial mixtures as $x_3(t) = (u + S_t)t = wt = n\lambda_{3x}/2$ and $x_1(t) = L_0 - x_3(t) = n\lambda_{1x}/2$, respectively. Then, the corresponding frequencies are $\nu_{3x}(t) = c_3/\lambda_{3x} = nc_3/2wt$ and $\nu_{1x}(t) = c_1/\lambda_{1x} = nc_1/2(L_0 - wt)$, i.e., the frequency of streamwise oscillations decreases with time in combustion products $\left(\frac{\partial\nu_{3x}}{\partial t} < 0\right)$ and increases with time in the initial mixture $\left(\frac{\partial\nu_{1x}}{\partial t} > 0\right)$. The resonance of the entire system

occurs when the frequencies coincide: $\nu_{3x}(t^*) = \nu_{1x}(t^*)$. The resonance occurs at the time determined by the relation $2c_1wt^* = c_3 \cdot 2(L_0 - wt^*)$, whence it follows that $t^* = [c_3/(c_3 + c_1)][L_0/w] < L_0/w$, i.e., earlier than the flame front runs over the entire length of the tube. As it follows from the last formula, the greater the visible velocity of the flame front $w = u + S_t$, the more rapidly the resonance occurs. A higher visible velocity of the flame front can be caused either by an elevated velocity of the normal flame S_u (as for hydrogen), or by natural or artificial turbulent fluctuations of the flow and turbulent velocity S_t , or an elevated mass velocity of the flow u . In the latter case, the flow velocity is determined by the initiator: the more powerful the initiator, the stronger flow of the mixture is generated by this initiator. It should be specially noted that the DDT refers to an intermediate regime of initiation of the mixture between its ignition by a "weak" source and "direct" initiation of detonation in an immediate vicinity of the initiator [8]. The difference in the critical energies of mixture ignition and detonation excitation is several orders of magnitude [8]. It should be emphasized that the laws concerning the DDT instant are confirmed experimentally. The coordinate at which the resonance occurs

is determined by the formula $x_3^* = c_3/(c_3 + c_1)L_0 < L_0$, i.e., it depends linearly on the tube length. As $c_3 > c_1$, the resonance occurs in the second half of the tube.

CONCLUSIONS

The result of coincidence of acoustic frequencies of vibrations in the initial mixture and combustion products is the resonance with a drastic increase in the amplitude of vibrations in the entire tube. It is this resonance that can initiate a transition from conventional to explosive combustion (instantaneous burning in a constant volume) with a significant increase in pressure in the explosion region. In turn, the drastic increase in pressure favors the formation of a powerful shock wave. When this wave reaches the bow shock wave, the parameters at the front significantly increase, the SW Mach number also noticeably increase, and a supersonic regime of wave propagation is reached.

This is the pattern of the deflagration-to-detonation transition, where the basic effect is the resonance of streamwise acoustic vibrations of the initial mixture and combustion products separated by the moving front of combustion in the flow of the combustible mixture. The simplest estimates of the resonance mechanism of the transition are consistent with available experimental observations.

REFERENCES

1. V. A. Mikhelson, "On the Normal Velocity of Ignition of Explosive Gas Mixtures," Uch. Zap. Imper. Mosk. Univ. Otd. Fiz.-Mat., No. 10 (Universitet. Tipografiya, Moscow, 1893) [in Russian].
2. K. I. Shchelkin and Ya. K. Troshin, *Gas Dynamics of Combustion* (Izd. Akad. Nauk SSSR, Moscow, 1963) [in Russian].
3. Ya. B. Zel'dovich and D. A. Frank-Kamenetskii, *Theory of Thermal Propagation of the Flame* (Nauka, Moscow, 1981) [in Russian].
4. J. Warnatz, U. Maas, and R. W. Dibble, *Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation* (Springer, Berlin, 1996).
5. N. M. Bazhun, V. A. Ivanchenko, and V. N. Parmon, *Thermodynamics of Chemists* (Khimiya-Kolos, Moscow, 2004) [in Russian].
6. D. V. Sivukhin, *General Course of Physics, Vol. II: Thermodynamics and Molecular Physics* (Nauka, Moscow, 1975) [in Russian].

7. *Physics of Explosion*, Ed. by L. P. Orlenko (Fizmatlit, Moscow, 2002) [in Russian].
8. A. A. Vasil'ev, "Cellular Structures of a Multifront Detonation Wave and Initiation (Review)," *Fiz. Goreniya Vzryva* **51** (1), 9–30 (2015) [*Combust., Expl., Shock Waves* **51** (1), 1–20 (2015); DOI: 10.1134/S0010508215010013].
9. *Tables of Physical Quantities: Reference Book*, Ed. by I. K. Kikoin (Atomizdat, Moscow, 1976) [in Russian].
10. L. D. Landau, "To the Theory of Slow Combustion," *Zh. Eksp. Teor. Fiz.* **14** (6), 240–244 (1944).
11. K. P. Stanyukovich, *Unsteady Motion of Continuous Media* (Nauka, Moscow, 1971) [in Russian].