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Abstract.

The article presents additional calculated data on combustion velocity for typical gas mixtures at pressures up to 6000 atm and temperatures up to 4000 K. It was determined that combustion velocity is mainly influenced by initial temperature, and the dependence on pressure is rather low. For fuel-oxygen and air-fuel mixtures in three-dimensional space (pressure–temperature–velocity of deflagration combustion), we have found a single surface of combustion velocities and continuous dependence of flame velocity on initial conditions.

Introduction.

One of the objectives of investigation of explosive risks of combustible systems is simulation of real scenario of all stages of explosion development: mixture inflammation and formation of low-velocity laminar flame, acceleration of flame front due to natural or artificial turbulization, formation of compression waves by the widening flame front, formation of compression shock by widening flame front, formation of weak shock wave (SW) and its subsequent intensification, explosive inflammation of compressed mixture (behind the SW front before the flame front), interaction of these non-stationary combustion fronts resulting under certain conditions in the rise of the detonation wave (DW). Most often DW emerges first in the area of gas compressed and heated with the shock wave, and then, after “overtaking” of the front of the bow SW by this wave in formation of DW in the initial mixture. The above described sequence of events is a typical scenario of deflagration to detonation transition (DDT).

The normal velocity of laminar combustion is determined by the processes of diffusion and thermal conductivity, and for their correct simulation it is necessary to have information on these coefficients dependence on the parameters of the medium continually changing during flame acceleration. It is obvious that there is a need not only in the physically substantiated models of flow turbulization, but in the change of main gas-dynamic parameters of the dependence of all main coefficients determining the process development that are correct for a wide range.

Until now the dependence of flame velocity W on pressure P and temperature T has been conventionally set in the form of empirical correlation (with larger degree of uncertainty)

$$W = W_{00}(P/P_{00})^n (T/T_{00})^m, \quad (1)$$

where the index 00 designates the values of parameters in some standard state, and the exponents n and m are determined on the basis of experimental data. Given relation is fundamental in the problem of flame acceleration and deflagration to detonation transition.

Approach.

The problem of functional dependence of combustion velocity W on pressure and temperature (formula of type (1)) may be approached taking into account the problem on the propagation of combustion and detonation waves in the reacting systems based on the laws of conservation of mass, momentum, and energy (for example, [1, 2]):

$$\begin{aligned} \rho_0 D &= \rho(D-u), \\ P_0 + \rho_0 D^2 &= P + \rho(D-u)^2, \\ I_0 + Q + D^2/2 &= I + (D-u)^2/2. \end{aligned} \quad (2)$$

Here ρ is mixture density (specific volume $V = 1/\rho$), P is the pressure, D and u are the wave and mass velocities, I is the enthalpy, and Q is the energy-release of mixture.

For better understanding briefly present the basic features of the work. As a result of algebraic transformations based on the laws of conservation of mass and impulse it is possible to obtain the Michelson—Rayleigh equation of a straight line (SMR) passing through the point of initial state (P_0, V_0)

$$\left(\frac{P}{P_0} - 1\right) = -\frac{\gamma_0 D^2}{c_0^2} \left(\frac{V}{V_0} - 1\right), \quad (2a)$$

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and from the energy equation (within the framework of the ideal gas model with heat capacity independent of temperature at constant volume

$$I = \frac{\gamma - P}{\gamma - 1 \rho} -$$

the adiabat of reaction products $P = f(V, Q)$ (energy release adiabat (EA)):

$$\frac{P}{P_0} = \frac{\frac{\gamma_0 + 1}{\gamma_0 - 1} \frac{V}{V_0} + 2\gamma_0 \frac{Q(P, V)}{c_0^2}}{\frac{\gamma + 1}{\gamma - 1} \frac{V}{V_0} - 1}, \quad (2b)$$

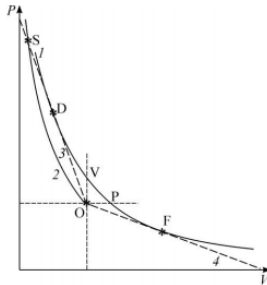


Fig. 1. Typical diagram of states of initial combustion mixture, reaction products, and its special points.

being a hyperbola in the (P, V) plane, convex towards the coordinate origin. Adiabatic exponents for initial mixture and reaction products are denoted by γ_0 and γ , respectively, energy release Q is considered constant on EA within the framework of idealized one-stage model or is a variable value along EA (function of system parameters) within the model of chemical equilibrium of the products. Figure 1 schematically presents SMR 3 and 4, shock adiabat 2 without energy release, adiabat of energy release I , and all characteristic points. On this EA, the detonation (at $P > P_0$ and $V < V_0$) and deflagration (at $P < P_0$ and $V > V_0$) branches are distinguished. Since point O of initial state lies beyond the hyperbola, from this point we may line rectilinear secants (both to detonation and deflagration branches of adiabat of energy release) with two cross points of this line with each branch of adiabat of energy release. Cross points collapse in one when the secant transforms into the tangent (self-sustaining wave of Chapman—Jouguet). A remarkable peculiarity of the system of equations for the description of combustion and detonation waves is that wave velocities complying with the condition of tangency of SMR 3 and 4 to detonation and deflagration branches are not arbitrary but turn out to be interrelated. This fact allows us to solve the problem.

Consider the detonation wave in relation to the point of initial state O. Shock wave transforms gas from the state O into the state S, complying with the chemical peak of DW, then chemical reaction starts, and after its completion, the reaction products get into point D. Transition from S to D is performed along Michelson line being tangential to the adiabat of energy release in relation to the initial state O. But Michelson line from O to S is simultaneously a tangent to adiabat of energy release lined from the point S, as initial [3]. It should be noted that adiabats of energy release built in relation to the points O and S, do not coincide with each other; only the condition and tangency point D remain. Isentropic line at the point D touches below the adiabat of energy release built relative to the point O, and touches the top of adiabat built relative to the point S. In other words, point D complies both with the parameters of detonation combustion relative to the initial state O, and the parameters of deflagration combustion with initial state at the point S. Note that already the classical works (for example, [1, 2]) expressed an idea that detonation may be presented as deflagration beyond the shock wave.

This view (from the point of detonation on combustion) allows analyzing the change of deflagration velocities in the states with different initial pressures and temperatures and even obtaining the analytical formula for the velocity of deflagration combustion depending on P_0 and T_0 . In the work [4], the state in the

chemical peak of the detonation wave was considered as initial state for the deflagration combustion in the flow of combustible mix beyond the shock front of DW within the model of ideal gas with constant Q and γ and, and the formula assessing combustion velocity depending on initial parameters of the mixture was obtained:

$$D_{FS} = D_{FO} \frac{\gamma_0 + 1}{2\gamma} \frac{\pi_S}{\sigma_S} = D_{FO} \frac{\gamma_0 + 1}{2\gamma} \frac{T_S}{T_0} \quad (3)$$

The latter formula, in addition, is the substantiation of a rather arbitrary formula (1).

Results and discussion

To verify the latter relation the parameters of combustion and detonation of stoichiometric mixtures of hydrogen and typical hydrocarbons (methane, ethylene, and acetylene, as representatives with single, double, and triple chemical bonds) with oxygen and air was calculated in approximation of chemical equilibrium at varying initial pressure in the range 0.001–100 atm and initial temperature in the range 200–1800 K, knowingly exceeding the areas of application [5]. The results confirmed the validity of the proposed formula (3), whereas the dependence on pressure was very weak. In addition, we calculated the parameters of combustion and detonation at initial state complying with the point S (simultaneous change of P and T). It should be emphasized that the condition $Q = \text{const}$ along the adiabat of energy release is a strong idealization, justified only by the possibility of simple algebraic transformation of the laws of conservation. Already in approximation of chemical equilibrium of the products, Q changes along the adiabat: for example, for the mixture $2\text{H}_2 + \text{O}_2$ at specific points of adiabats $Q_D = 972.6$, $Q_V = 1057.5$, $Q_P = 1117.6$, and $Q_{DF} = 1199.7$ cal/g. If we select the state at the point S as initial, then at point D, being the deflagration point, $Q_{DF} = 1580.4$ cal/g. Comparing with the value Q for the point D as detonation point relative to the state O ($Q_D = 972.6$ cal/g), note that these values considerably differ (see above mentioned on non-coincidence of adiabats of energy release for the points O and S).

It should be noted that the parameters of the point S as the initial state are not included in the initial regular grid of pressures and temperatures $\{P_0, T_0\}$, since limited by the frameworks of the laws of conservation. There is a logical question whether the velocities of deflagration combustion for irregular initial conditions fit on some surface of velocities built on the grid with regular data. In other words, whether the surface of combustion velocities is single for arbitrary initial data. In the language of mathematics, the existence of a single surface means continuous dependence of the solution on initial conditions. Use of the point S as the point of initial condition widens the range of temperatures to 4000 K, and the range of pressures — to 6000 atm.

As was noted above, the dependence of combustion velocity D_{FO} on initial parameters $\{P_0, T_0\}$ forms the surface of combustion velocities in three-dimensional space $\{P_0, T_0, D_{FO}\}$. It turned out that combustion velocities D_{FS} in relation to the state S with increased irregular parameters $\{P_S, T_S\}$ also belong to the surface $\{P_0, T_0, D_{FO}\}$ of combustion velocity formed by regular initial grid $\{P_0, T_0\}$. This is illustrated by figure 2, for example, for air-hydrogen mixture (air-fuel mixtures). In the figure there is the common surface for different groups of data: $\{P_0, T_0, D_{FO}\}$, and $\{P_S, T_S, D_{FS}\}$. Combustion velocities surfaces of other mixtures (oxygen-hydrogen, air-acetylene, air-methane etc.) have the same feature. This proves the existence of a single surface of combustion velocities for different propagation modes. In other words, we observe the continuous dependence of solution (flame velocity) on initial conditions.



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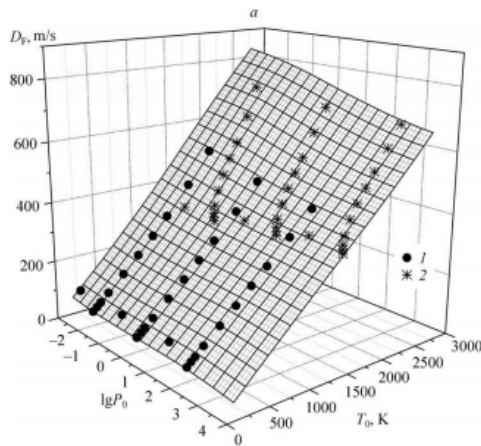


Fig. 2. Surface of combustion velocities for the mixture of hydrogen with air.
 1 — D_{F0} , 2 — D_{FS} .

Conclusions.

Thus, in this work there are additional calculated data on combustion velocity for typical gas mixtures at pressures up to 6000 atm and temperatures up to 4000 K. It was found that mainly the combustion velocity is influenced by initial temperature, and dependence on pressure is rather weak. Combustion velocities D_{F0} for oxygen-fuel and air-fuel mixtures depending on initial parameters $\{P_0, T_0\}$ form a single surface in three-dimensional space $\{P_0, T_0, D_{F0}\}$, that proves a continuous dependence of solution (flame velocity) on initial conditions.

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