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OTS: 60-11,728

JPRS: 2785
6 June 1960

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DETONATION PROCESSES

- USSR -

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Distributed by:

OFFICE OF TECHNICAL SERVICES
U. S. DEPARTMENT OF COMMERCE
WASHINGTON 25, D. C.

Price: $0.50

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205 EAST 42nd STREET, SUITE 300
NEW YORK 17, N. Y.

JPRS: 2785

CSO: 3939-N/a

DETONATION PROCESSES

[This is a translation of an article by K. I. Schelkin, Corresponding Member Acad. Sci. USSR, in Vestnik Akademii Nauk SSSR (Herald of the Acad. Sci. USSR), No. 2, 1960, pages 12-20]

At the end of the last century, catastrophic explosions in coal mines prompted scientists of various countries to undertake detailed investigations of the propagation of flame in gases.

The gas detonation -- the propagation of combustion with a uniform supersonic velocity which is of the order of 2 to 3 km per second and quite definite for a given combustible mixture -- was an important scientific result of these researches discovered in 1881 by four French chemists (Mallard and Le Châtelier, and, working independently, Berthelot and Vieille). Since that time, this interesting and complex phenomenon, which is unknown under purely natural conditions and had its genesis in the development of technology, has been investigated with success by scientists of various countries.

The investigators addressed themselves at once to the question as to what physical process causes combustion to advance at such a high velocity. Heat conduction and diffusion, which govern the propagation of slow-moving flames, could not account for the supersonic velocities of the detonation. Mallard and Le Chatelier found the right track in assigning the principal role in the propagation of detonation-type combustion to compression of the gas.

The classical theory of detonation, which is based on the theory of shock waves, is due to the Russian physicist V. A. Mikhel'son, who published it in 1890. However, Mikhel'son's work remained unknown abroad, and the English scientist Chapman worked out a theory of detonation independently 9 years later.

The basic points of his theory are as follows. In the detonation wave, as in the shock wave, the gas is compressed sharply. Moreover, due to its sharpness, shock compression heats the gas more strongly than adiabatic compression. With an unlimited pressure increase in the shock wave, the ratio of the density of the gas to the initial density (the compression ratio) tends to a finite value which, for an ideal gas, is proportional to its heat capacity. Here the limiting relative compression is four for a monatomic gas and six for a diatomic gas.

The distribution of pressure (density, temperature) in the detonation wave is indicated in Fig. 1. To describe a detonation it is necessary to find 5 unknown quantities: the velocity D of the front and the pressure, density, temperature, and velocity of the products of combustion. The initial state of the mixture (pressure, density, and temperature), its heat of combustion, and the heat capacities of the unburned gas and the products of combustion are regarded as knowns. Three equations are written to define the unknowns: the equations of conservation of mass, momentum, and energy in the passage of the gas through the wavefront AB. In a departure from shock-wave theory, the heat of combustion is taken into account in the equation of conservation of energy. The equation of state of the products of combustion serves as a fourth equation; for gases, this is usually the equation of Clapeyron.

Four equations are, of course, insufficient for the determination of five unknowns. Since a fifth equation was lacking, they were restricted to the calculation of four quantities, although a fifth, e.g., the velocity of the detonation, was assigned.

In Fig. 2, the curve H (the Hugoniot curve, after the author of the theory of shock waves) indicates the pressure of the products of combustion as a function of their specific volume -- the reciprocal of the density ($v = 1/\rho$), and curve 1 characterizes the analogous relationship in the shock wave (for the unburned gas). The velocity of the detonation is determined by the slope (to the $\frac{1}{2}$ power) of the straight line passed from A to the point with the value of the pressure in the detonation wave. As will be seen from Fig. 2, the laws of conservation of mass, momentum, and energy assume the existence of a continuous spectrum of detonation velocities from a minimum value defined by the tangent AB to infinity, since as many straight lines as we please may be drawn from A between AB and the vertical to intersect the curve H.

To find a fifth equation meant to find a method of selecting a single velocity value from the continuous spectrum. Many intuitively gave preference to the velocity determined by the tangent AB, but no one was able to demonstrate the correctness of this choice.

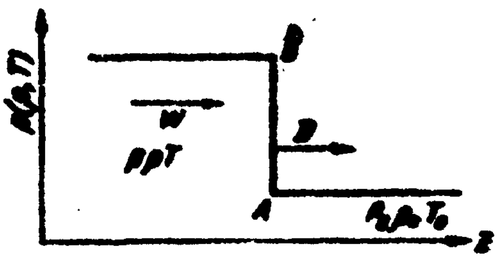

Fig. 1. Diagram of detonation wave. p_0, ρ_0, and T_0 are the pressure, density, and temperature of the initial gas; p, ρ, and T are the same values for the products of combustion, D is the velocity of the detonation front AB, and w is the velocity of the products of combustion.

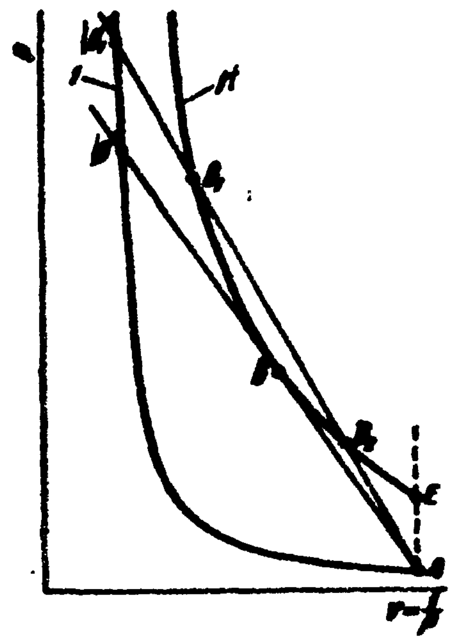

Fig. 2. p-V diagrams; 1--for shock wave; 2--for products of detonation; A--initial point for both curves.

Finally, the French investigator Jouguet noted a highly important singularity of the point B. In the state B, the velocity of the wavefront relative to the products of combustion is exactly equal to the velocity of sound therein. For all other points of the curve H lying above B, the velocity of the wave is lower than the velocity of sound. This property of point B leads to an important result: the rarefaction wave which appears behind the detonation front does not overtake it; it moves through the products of combustion at the velocity of sound, but the front moves out ahead of it with the same velocity. On the other hand, a detonation with a pressure higher than that at point B will be attenuated by rarefaction waves which overhaul its front until the pressure is reduced to the value at point B. Rarefaction always occurs behind the front in a tube, even when the products of combustion are not cooled. The gas in the detonation wave is displaced in the direction in which its front moves; rarefaction will therefore appear somewhere to the rear, whence the gas has departed. This may be eliminated by compressing the products of combustion by some method, e.g., by a piston, the overpressure detonation will then become stable. In the case considered here -- that of free propagation of the detonation -- only the state at the point B will be stable.

Thus the fifth equation, which is termed the condition of choice of velocity or the Jouguet condition, proved quite simple: the velocity of the wave with respect to the products of combustion is equal to the velocity of sound in them. The theory had been completed; all five unknowns were now determined from the initial data.

But the triumph was still not complete: it remained unclear why the states lying on the lower section of the Hugoniot curve between the points B and E were not realized.

The solution to this problem, as is often the case in science, required a new elucidation of the entire problem.

It had been assumed previously that the gas passed instantaneously from the state A (Figs. 1 and 2) into the state B. However, as was correctly noted by Ya. B.

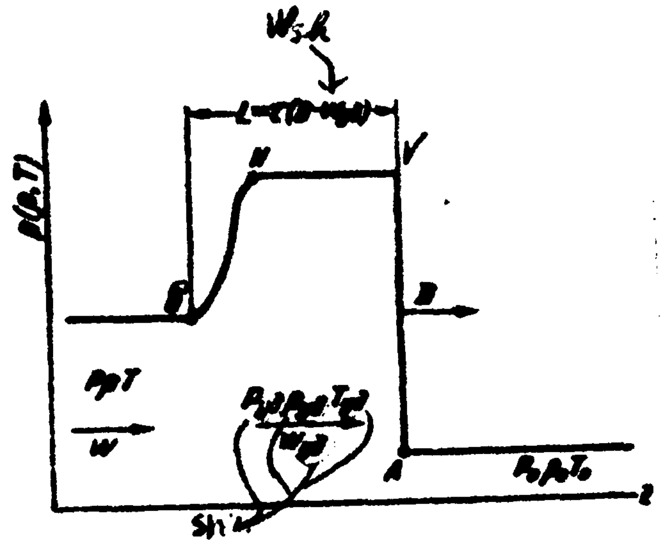

Fig. 3. Diagram of detonation as a shock-wave/reaction-zone complex.
L--width of reaction zone; τ--time of reaction. As a result of the heavy (exponential) dependence of the rate of reaction on temperature, the liberation of energy occurs over the small segment NC.

Zel'dovich (1), combustion does not begin instantaneously and requires a certain time τ . Thus there exists in front of the products of combustion a zone of compressed and heated but as yet unreacted mixture whose forward boundary, the shock-compression front, is moving with the velocity of the detonation. The state of the compressed mixture

(1) See, for example, Ya. B. Zel'dovich and A. S. Kompaneyets, The Theory of Detonations, M., 1955.

must occur simultaneously on the curve 1 and on the extension of the line AB, i.e., at the point of intersection C (Fig. 2). The distribution of pressure in the detonation wave should therefore be complemented by a zone of elevated pressure CNB, as represented in Fig. 3. The shape of the curve CNB depends on the course of the chemical reaction, which determines the amount of energy liberated. Ya. B. Zel'dovich computed the distribution of the pressure, density, and velocity of the gas in the zone CNB for various cases of the chemical-reaction process. He developed a method by which the velocity of the detonation and the motion of the products behind its front could be calculated in the presence of an energy loss, e.g., through friction in the zone of chemical reaction.

Having refined the structure of the detonation wave, it is easy to understand the explanation proposed by Ya. B. Zel'dovich for the impossibility of states on the segment BE (Fig. 2). To realize the state B_2, for example, the gas must pass the point B_1 after dropping from A to C_1 and then move along the straight line to the point B_2. We say along the straight line because all parts of the wave move with the same velocity, which is determined by the slope of the straight line AC_1. But states lying on the line between B_1 and B_2, inasmuch as they lie above the curve H, require larger liberated energies than those in our mixture, which is described by the curve H. In other words, an energy barrier which the gas has no reserve of energy to overcome is found on the straight line between B_1 and B_2, when ignition is produced by shock compression. Therefore the states B_2 and other points on the segment between B and E are unattainable and are not realized. These states, which correspond to the underpressure detonation, may be obtained by igniting a mixture with a specified velocity, e.g., by a multitude of low-energy spark discharges. The simultaneous discharge in all spark gaps, which simulates an infinite velocity of propagation of the combustion, may be described by the state at the point E, which corresponds to combustion at constant volume. In this case the velocity of the products of the reaction is zero.

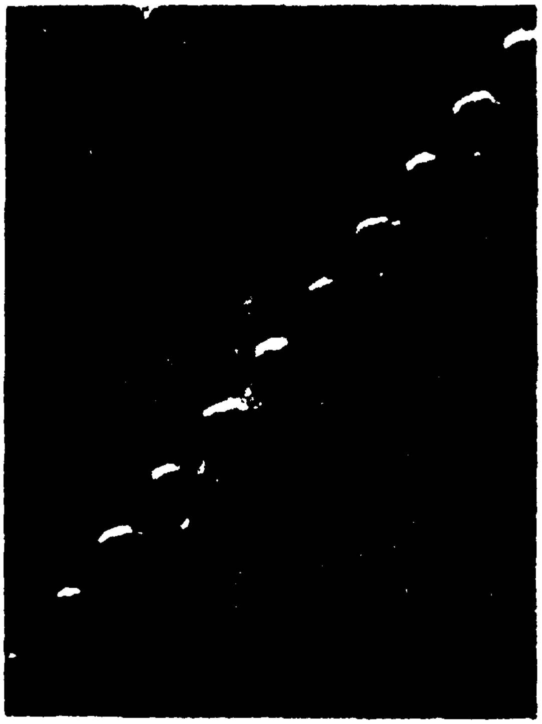

Fig. 4. Photograph of spin detonation on moving film. The wave is being propagated from right to left.

Fig. 5. Trace of motion of normal detonation on moving film.

Thus was the classical theory of detonations perfected. Developed for gases, it is applied successfully to detonations of condensed explosives -- being propagated, incidentally, with velocities up to 8 kilometers and more per second and characterized by pressures of the order of 100 to 200 atm in the front. The reliability of the calculations for explosives was improved after the derivation by L. D. Landau and K. P. Stanyukovich of a theoretically-based equation of state for the products of the explosion that supplanted the numerous empirical formulas.

The theory of detonations appeared exhaustive. Yet an experimental fact existed which did not fit the scheme of the plane detonation. In 1926, in a mixture of carbon monoxide and oxygen, the Englishmen Campbell and Woodhead observed the spin detonation, in which the initiation is concentrated in a nucleus which, simultaneously with its forward motion, revolves about the axis of the tube (the spin) thereby describing a spiral with a step approximately equal to three diameters of the tube. The zone of combustion, which occupies the entire cross-section of the tube for a length equal to one to three of its calibers, is drawn behind the nucleus like the tail behind the head of a comet. A trace of the motion of a spin detonation on a moving film reveals the wavy front line and the characteristic banded structure of the afterglow (Fig. 4). It differs sharply from the normal (nonspin) detonation shown in Fig. 5.

Spin was shortly thereafter detected in other slowly-reacting mixtures as well. Kh. A. Rakipov, Ya. K. Troshin, and K. I. Shchelkin obtained spin detonation in a typical nonspin mixture of hydrogen with oxygen by employing various methods to approach the limits of propagation of detonation in them: either by enriching or impoverishing the mixture in hydrogen, or by reducing the diameter of the tube, or by lowering the initial pressure. This much was clear: the detonation acquires a spin character in any mixture when the ratio of the width L of the chemical-reaction zone to the diameter of the tube is increased to a certain value (Fig. 3).

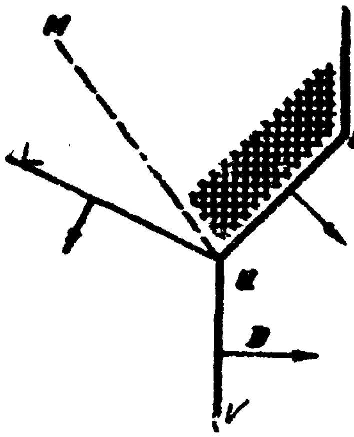

Fig. 6. Diagram of oblique detonation shock. VI--shock wave moving with velocity of detonation; IK--oblique shock; shaded area--zone of initiation; IL--weak shock wave; IM--tangential velocity discontinuity.

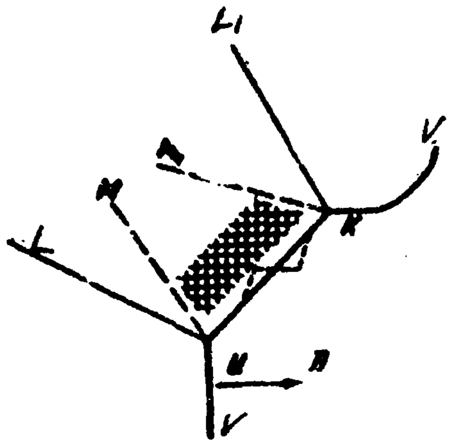

Fig. 7. Symmetrical oblique detonation shock. KL_1--shock wave; KM_1--tangential discontinuity (other designations same as in Fig. 6).

The author of the present article was able to show (1) that the spin nucleus is an oblique (broken) shock wave in which the mixture is ignited more readily than in a plane wave, since the temperature and pressure in it are significantly higher. The oblique wave appears as a result of the instability to disturbances shown by the complex consisting of the shock wave and the initiation zone which follows it (Fig. 3). When the extent of the oblique shock,

(1) See K. I. Shchelkin, Rapid Combustion and Spin Detonation in Gases, M., 1949.

which is proportional to the width of the reaction zone in the plane wave, is comparable to the radius (diameter) of the tube, a single-headed spin appears; an increase in the tube diameter or a reduction in the width of the reaction zone makes room for two or more oblique shocks in the tube section, and a two-(or multi-) headed spin arises. The spin may be eliminated by directing the spin detonation into a severely rough-surfaced tube. Zones of elevated temperature -- local ignition foci -- arise at the points of reflection of the wavefront AC (Fig. 3) from the roughened surface, initiation is transferred entirely from the zone NB to the plane AC, the detonation front is stabilized and the spin vanishes. In addition, the velocity of the detonation is lower in a rough-walled tube than in a smooth-walled tube; as a result of its dependence on apparatus factors, it loses its nature as a physicochemical constant of the mixture in the rough-walled tube.

Figure 6 gives a diagram of the oblique detonation. Its configuration accounts for the characteristic structure of the afterglow; in particular, the shock wave IL serves as the originator of the almost horizontal bands (Fig. 4).

As attractive as this explanation of the spin detonation might have seemed, especially to the author, it had a weak point. The oblique detonation is propagated with respect to the undisturbed gas at a velocity significantly ($\sim$ 1.4 times) higher than the plane detonation. Therefore the state which prevails therein is represented in Fig. 2 by a point lying above the point B. Why, then, doesn't the oblique wave fade? We know that according to Jouguet, such a wave must inevitably fall off in intensity until its state has dropped to the point B.

Ya. B. Zel'dovich remedied this difficulty. He showed that in an oblique detonation which occupies only part of the section of the tube, the products of combustion are compressed by the surrounding unburned gas in the remaining, larger part of the cross section. The oblique detonation is therefore a stable overpressure wave; there is no rarefaction behind its front capable of attenuating it, at least as long as the combustion behind the oblique wave fails to overtake it and remains within the limits of the high-pressure region VN (Fig. 3).

Sufficient basis has been found for the description of the spin detonation as a detonation driven by an oblique compression shock. However, the details of the oblique shock's structure have not yet been fully clarified. In particular, the angle K (Fig. 6) may possibly take the form represented in Fig. 7, as suggested by Yu. N. Denisov and Ya. K. Troshin.

The general question arises as to whether the classical theory of the plane detonation is at all applicable to the spin detonation. In composing the equations of conservation, it is formally possible to write them for the initial and final states without considering the zone in which initiation, having started in the oblique shock, will be propagated over the entire cross section of the tube. Here the shock wave IL and the transverse vibration of the gas to which it gives rise are not taken into consideration; turbulence in the tangential discontinuities IM is also neglected (Figs. 6 and 7). This method may be used to calculate approximately the velocity of the spin detonation (the results coincide satisfactorily with experiment) and determine the state and velocity of the products of combustion, but yields virtually no conclusion concerning the reaction zone. Calculation of the spin detonation's reaction zone as a three-dimensional process is inordinately difficult. The problem is vastly simplified when converted to two dimensions by unrolling the spiral motion onto a plane, as indicated in Fig. 6. The angle between the waves VI and IK (Figs. 6 and 7) has a definite value for a specified liberated energy. Knowing the velocity of the front VI from classical theory, we may find the velocity of the boundary IK from the angle between VI and IK, and then determine the corresponding point of the type B_1 on the curve H (Fig. 2) and find all remaining unknowns in all regions on Fig. 6.

Let us return to the front structure of the normal detonation. As noted by Yu. N. Denisov and Ya. K. Troshin (1), the collision of two normal detonation waves leaves a winding track on the blackened surface of the tube. The mark due to the collision of a normal detonation with a plane shock wave is also nonuniform; only two shock waves produce the ideal straight line upon mutual reflection. The normal detonation leaves a reticulated pattern on the blackened wall (Fig. 8); this indicates motion across the surface of the detonation front of numerous disturbances which are reflected from one another and give rise to amplifications of the wave and pulsations of the combustion zone at the points of encounter. By distorting the surface of the detonation front, these disturbances, which are minute oblique waves, produce the uneven track left by the collision of two detonations or the collision of a

(1) See Yu. N. Denisov and Ya. K. Troshin, "Proceedings of the Academy of Sciences USSR," 1959, Vol. 125, page 110.

detonation with a plane shock wave. The size of the cells increases as the limit of detonation is approached. In short, everything occurs as in the spin with the sole difference that many oblique shocks are arrayed over the section of the tube; the diameter of the tube is large by comparison with the width of the reaction zone. Having no preferred direction of motion, these shocks collide; the mixture ignites at the points of encounter

Fig. 8. Track of "normal" detonation on blackened surface of tube. The wave is propagated from right to left.

even more readily than in the oblique shocks, the surface of the front acquires the form of a brush and the front pulsates.

As a result of these experiments, the authors of the present paper were brought back to the problem of the instability of the plane detonation wave (1).

Approximate quantitative analysis led to the following criterion for the loss of stability of a plane detonation:

$$\frac{E}{RT}\left[1-\left(\frac{p_B}{p_V}\right)^{\frac{\gamma-1}{\gamma}}\right]\geqslant 1. \qquad (1)$$

where E is the activation energy of the combustion reaction, T is the temperature in the region VN, p_B and p_V are the pressures at the corresponding points of the curve H, and γ is the ratio of the heat capacities.

The following reasoning will help qualitatively in clarifying the cause of the instability. Suppose the time of the combustion reaction for some volume of gas occupying part of the tube section is found to be longer than τ (Fig. 3). Then this volume, having reached the zone to the left of B, where the pressure is lower, will expand laterally and cool, and its combustion time will increase still further. On the other hand, an element which has begun to react earlier than the others will be compressed and react even more rapidly, since it is subject to the conditions of the overpressure detonation. The arbitrary disturbance of the zone BN (Fig. 3) increases, and it is this that constitutes instability.

Approximate calculations (exact calculations are extremely laborious) by Formula (1) indicate instability of the plane detonation in typical combustible mixtures. Consequently, the pulsating structure of the front of the "normal" detonation should be quite common.

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(1) See K. I. Shchelkin, "Journal of Experimental and Theoretical Physics," 1959, Vol. 36, page. 600.

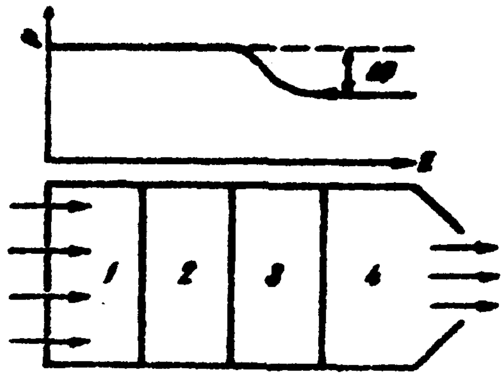

Fig. 9. Simplified diagram of rocket combustion chamber.
1 and 2 -- zones where fuel is mixed with oxidizer and mixture is preheated; 3 -- reaction zone; 4 -- products of combustion.

Let us return to the single-headed spin and consider segment IK of the oblique shock (Figs. 6 and 7). This a plane overpressure detonation which, if the criterion is greater than unity, should also lose its stability. n disturbances (minute oblique shocks) must necessarily ear in it, as indicated by the broken lines in Fig. 7. N. Denisov and Ya. K. Troshin did indeed detect fine ucture of the nucleus of a single-headed spin, indicag the motion of minute disturbances across it.

The instability of the plane wave increases the tality" of the detonation -- if we may use such an ression -- by creating zones in which the temperature higher than in the plane wave; these are reliable ination foci. The instability of one form of detonation ngs new, more stable fôrms into existence.

Where is the limit? Will not a small oblique shock g. 7) give rise, for example, to its own still smaller oblique waves? A limit does, of course, exist. First of all, the value of the criterion (1) decreases as the intensity of the wave (its temperature in the zone V, Figs. 2 and 3) increases, and stability may set in. But there is also a nontrivial limit. The very short reaction times are determined by the excitation period of the fuel-molecule vibrations. The dependence of the reaction time on temperature ceases to be exponential -- the time approaches a finite value -- and all conclusions concerning instability lose their force. From this is follows that the size of the oblique shock cannot be too small. The minimal reaction time in explosive substances with complex molecular structures and in hydrocarbons containing large numbers of atoms probably amounts to fractions of a microsecond. An investigation of the structure of the detonation and the stability of its front in such substances would be highly interesting in many respects.

The skeptic may ask, why all this hair-splitting? Of what practical value are the structural details of detonations -- especially those of the gas detonation, which isn't applied in a single technological process?

In lieu of a reply, let us present certain results of application of the theory of detonation to a phenomenon which would appear to be quite remote from it -- i.e., to combustion in a rocket chamber, a process profoundly analogous to the detonation (1).

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(1) See Yu. N. Denisov, Ya. K. Troshin, K. I. Shchelkin, "Bulletin of the Academy of Sciences USSR, Division of Technical Sciences, Power Engineering and Automation," 1959, No. 6, page 79.

Without plunging into detail, let us assume that as in a plane detonation (Fig. 3), the gas in zone 3 of the rocket chamber (Fig. 9) is ignited successively (an assumption which is not always justified). Then, applying Formula (1), we may obtain the criterion for the appearance of high-frequency combustion pulsations in the chamber:

$$(\gamma - 1)^2 \frac{E}{RT} \frac{M^2 Q}{c^2} > 1, \qquad (2)$$

where M is the Mach number in zone 2, c is the velocity of sound therein, and Q is the heat of combustion per unit of mass. The criterion (2) is derived from (1) with the aid of the detonation equations by neglecting the squares and products of $\Delta p/p$ and M and regarding Q/c^2 as large by comparison with unity.

How astounding are the unexpected applications of science! Without overstatement of its practical significance, the example of the rocket chamber may be said to reaffirm this old adage once again.

Unfortunately, the scope of this paper does not permit us to go into the analogy between detonation and combustion in the chamber; nor does it allow treatment of the transition of slow combustion into detonation, the limits of the latter's propagation, detonations in rough-walled tubes, the propagation of explosions in air-and-powder mixtures, and the like. This fascinating field of science concerned with combustion and explosions, which contains an interwoven multitude of processes of various types, is uncommonly broad and many-faceted.

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