Journal of Propulsion and Power
Vol. 22, No. 3, May–June 2006

To the Question of Energy Use of Detonation Combustion

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Translation of article originally published in Russian in Zhurnal tekhnicheskoi fiziki (Journal of Technical Physics) 10 (17), 1940, pp. 1453–1461

DURING detonation combustion[1] of explosive gas mixtures, immediately after the passing of detonation wavefront (completion of chemical reaction), the products of combustion are in a state (call it state D) that is quite rich in both heat and kinetic energy (i.e., the energy of translational motion).

Assuming no losses, the state D of combustion products can be calculated using the classical thermodynamic theory of Jouguet. The propagation speed of detonation obtained in this calculation agrees well with experiment, which confirms the correctness of the thermodynamic theory as the limiting case with no losses.

For the combustion products in the detonation wave, such a calculation gives: density is 2–1.7 times greater than that of the initial mixture (approximately $(k+1)/k$ times greater, where k is the adiabatic exponent, $pv^k =$ const, for the combustion products); pressure is approximately 2 times greater than the pressure achieved in a closed-volume explosion; temperature is 10-20% higher than the temperature of a closed-volume explosion (approximately $2k/(k+1)$ times higher); speed of translational motion is about 0.4–0.5 times that of detonation propagation, which means that kinetic energy of translational motion reaches 17% of the total energy of the mixture.

It is interesting to consider to what extent detonation combustion of fuel allows more efficient energy use. One often comes across proposals for detonation regime of combustion in machines such as a gas turbine. Below we present a thermodynamic analysis of the efficiency of cycles with detonation. We will consider here the essential aspects and only briefly comment about technical viability of cycles, losses that reduce the efficiency as compared to the calculated values, etc.

1. Energy Balance in Detonation

We will establish that the cycle calculation that is based on the state (D) right after combustion (the state to which the above numbers refer) would be incorrect. In fact, consider a process in which the detonation combustion products in state D first decelerate, loosing their kinetic energy, and then expand from pressure $p_D \simeq 2p_{\text{explosion}}$ to the atmospheric pressure, doing work. We then arrive at a contradiction to the energy conservation law.

As a matter of fact, the total energy of working fluid in this calculation method is always greater than the energy (thermal and chemical) of the initial mixture. Obviously the combined thermal and chemical energy of the quiescent initial mixture is equal to the energy of products, also at rest, of a closed-volume explosion in which no work has been done. However, right behind the detonation wave front, the combustion products are both at a higher temperature than in a closed-volume explosion (i.e., they have greater thermal energy) and also moving with substantial kinetic energy.

Where does the extra energy come from? In reality, the total energy after detonation of a gas volume cannot differ from the initial energy, but can only be redistributed to some extent. If a part of the matter attains a more energetic state D, it may happen only at the expense of reduced energy of some other part of the detonation combustion products. In fact, the excess of energy of newly burned substance in state D is just due to the expansion and deceleration of the part of the substance that has been burned earlier. Therefore, not all the energy of deceleration and expansion of the product in state D can be used to perform external work because a part of this energy must be used to reproduce state D in subsequent portions of gas. We need other methods to determine maximum external work—see Section 2. The necessity for the reaction products to expand and decelerate after state D follows obviously from the fact that the density in state D is higher than the initial density and the velocity is in the direction of the detonation propagation. The spatial distribution of density, shown in Figure 1, and the corresponding distributions of pressure, temperature, and velocity (the latter is zero at segment AB) follow—in absence of any losses, such as heat transfer or hydraulic resistance of the tube—from the equations of rarefaction waves[2] and the Jouguet condition, which states that the sum of the speed of sound and the speed of the fluid's motion in state D is equal to the propagation speed of the detonation. Point B divides the entire distance AC traveled by detonation approximately in the proportion $AB{:}BC = 4{:}6$. As the process develops (detonation propagates) to the right, each specific elementary mass goes through the entire sequence of states shown in Figure 1, from the the initial state shown in the segment from C to ∞ to the post-expansion state in segment AB. The density dlstribution derived by Langweiler[3] contradicts Zemplen's theorem, according to which the rarefaction wave cannot propagate as a strong discontinuity, and therefore is incorrect.

If we wanted to keep all the burned matter in state D, we would have to move a piston with the speed equal to the speed of motion of reaction products in state D, i.e., approximately 0.43–0.47 times the propagation speed of detonation. In Figure 2 depicting such a thought experiment, $AB{:}AC = 0.45$. We should subtract the work done by the piston from the work, calculated above, that could be done by a unit mass of combustion products in state D. In the experiment of Figure 2, it is the work done by the piston (rather than the work of expansion and deceleration of reaction products behind the wave, as in the experiment of Figure 1) that is the source of excess energy in state D as compared to the energy of the initial mixture. On the contary, in the system of coordinates moving together with the detonation wave,[4] the piston (that moves slower) moves to the left of the wave and gains the work performed by the combustion products. The source of excessive energy in a state in this system of coordinates is the enormous kinetic energy of fresh mixture that moves in this system towards the wave with the speed of propagation of the detonation. Therefore, in order to clearly understand the relations in the detonation wave, we need to know the laws of transformation of the energy equations to a moving system of coordinates. These laws are well illustrated by a known problem: A passenger in a train moving with speed v_0 imparts a speed v_1 (relative to the train) to mass m. In the passenger's opinion, he has done

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[1] References to the literature are presented in the detailed work Ya.B. Zeldovich *Journal of Experimental and Theoretical Physics*, Vol. 10, No. 5, 1940.

[2] See, for example, Zeldovich and Shchelkin, *Journal of Experimental and Theoretical Physics*, Vol. 10, No. 5, 1940.

[3] Langweiler *ZS. f. techn. Phys.*, **19**, 277, 1938.

[4] It is convenient to derive equations in the moving system of coordinates where the process is stationary.

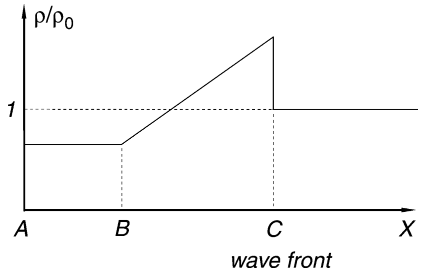

Fig. 1

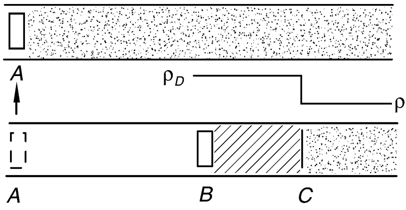

Fig. 2

work $m\mathrm{v}_1^2/2$, whereas according to a stationary observer, the work is equal to

$$m(\mathrm{v}_0+\mathrm{v}_1)^2\big/2-m(\mathrm{v}_0)^2\big/2=m(\mathrm{v}_1)^2\big/2+m\mathrm{v}_1\mathrm{v}_0$$

Where does the extra energy $m\mathrm{v}_1\mathrm{v}_0$ come from?

2. Efficiency of Cycle with Detonation Combustion

We could calculate the efficiency of such a cycle as a whole considering either the distribution of Fig. 1 or the thought experiment of Fig. 2, taking into account the work done by the piston.

However, we will choose here a somewhat different approach, which reflects the limiting values of the numbers derived below (in the absence of any losses) in terms of no possibility to surpass them using various engineering tricks. In the final state, after performing work, the combustion products attain the pressure $p_0=1$ kgf/cm^2. After subtracting the work $p_0(v-v_0)$ done against the force of the external pressure, the available work is equal to the difference between the initial heat content J_0 (heat content is defined as $J=E+pv_0$ and includes the chemical energy of the mixture, $J_0=J_0'+Q$) and the heat content of the reaction products J:

$$A=J_0-J=J_0'+Q-J$$

The heat content of the reaction products becomes fully determined if one specifies the entropy of the fluid S in addition to its pressure $p=p_0=1$ kgf/cm^2. If the process of doing work is ideal, the entropy remains constant after combustion (chemical reaction). Any increase in the entropy implies an increase in the heat content $J(p_0,S)$ and a decrease in the amount of work performed.

The thermodynamic theory of detonation considers all states that satisfy three conservation laws—of matter, momentum, and energy—for various propagation speeds of this regime (see curve H on the p–v plane of Fig. 3). It turns out that minimal entropy is attained exactly at point D (state D), which corresponds to the stationary propagation of the detonation satisfying the Jouguet condition mentioned above.

It is well known that a line from point O, which represents the initial mixture, to point D touches the Hugoniot adiabatic curve H at point D and also touches the isentropic curve (Poisson adiabatic curve) that passes through the same point D, as shown by the dash-dot line in Fig. 3. To the right of point D, the slope of curve H is less than that of the curve of constant entropy.

3. Entropy at Point *D* is Less than Entropy of Products of Constant-Volume Combustion (Point *E*)

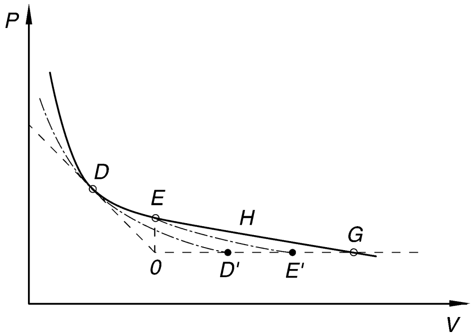

Fig. 3

Correspondingly, the reaction products that have done work after detonation (point D' in Fig. 3) have less energy than the reaction products that have expanded and done work after a closed-volume explosion. Point E on curve H in Fig. 3 represents the state of products of a closed-volume explosion. The point E', which represents the state of these products after they have done work, is the intersection of the curve of constant entropy, drawn from point E, with the line $p=p_0=1$ kgf/cm^2. Point E' lies to the right of point D', and therefore has a higher energy content. Finally, point G represents the results of combustion under constant pressure that is obtained without external work other than the work against the atmospheric pressure. At point G, we have $A=0$; $J_G=J_0=J_0'+Q$. Using J_G, the efficiency of the cycle can easily be written as

$$\eta=\frac{A}{Q}=\frac{J_0-J}{J_G-J_0'}=\frac{J_G-J}{J_G-J_0'}$$

Here is the simplest numeric example to illustrate these relations. An explosive mixture reacts with no change in the number of molecules (e.g., for ethylene, $C_2H_4+3O_2=2CO_2+2H_2O$). The specific heats of the reaction products are $c_p=7$ and $c_v=5$; the adiabatic exponent is then 1.4. The heat of the reaction is 10500 cal/mol. The initial temperature is 300 K. During the combustion at constant pressure, the temperature reaches $300+10500/7=1800$ K. The constant volume explosion of such a mixture results in a final temperature of $300+10500/5=2400$ K. The pressure is $1\cdot 2400/300=8$ kgf/cm^2. During the constant-entropy expansion from 8 to 1 kgf/cm^2, the temperature drops to $2400\cdot 8^{-0.286}=1330$ K. Ideally, the cycle in which the mixture explodes in a closed volume without pre-compression and the explosion products then expand to 1 kgf/cm^2, has an efficiency of

$$\eta_B'=\frac{(1800-1330)7}{(1800-300)7}=\frac{470}{1500}=0.313$$

During detonation combustion (in state D), the pressure reaches 15.55 kgf/cm^2. The specific volume decreases to 0.6 of the initial value. Temperature reaches 2800 K. The kinetic energy of the combustion products is 0.167 times the reaction heat of the mixture.[5] During the isentropic expansion to 1 kgf/cm^2, the temperature drops to $2800\cdot 15.55^{-0.286}=1270$ K. According to the argument above, the efficiency of a lossless detonation combustion appears to be equal to

$$\eta_D=\frac{1800-1270}{1800-300}=0.354$$

Therefore, detonation combustion can in principle result in somewhat more efficient use of fuel energy compared to the explosion in closed volume: $\eta_D=0.354$ versus $\eta_B=0.313$, i.e., with improvement of 13%. Of course, precompressing the explosive mixture increases the efficiency of both processes; at the same time, the difference $\eta_D-\eta_B$ decreases.

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[5] These figures have been calculated exactly. The formulas for the limiting case in which we neglect the thermal energy of the initial mixture with respect to its reaction heat would yield $p=16$ kgf/cm^2, $v=0.584$, $T=2800$ K, and kinetic energy equal to 1/6 of the chemical energy. These numbers are quite close to the exact.

Note, finally, that a naïve calculation of work that could be done by gases in state D (neglecting the work necessary to sustain the detonation wave) would yield an efficiency of 0.689. This number is the sum of the kinetic energy of the combustion products, 0.167 Q, and the work done during their expansion (from the state with $T = 2800$ K, $p = 15.55$ kgf/cm^2 to the state with $T = 1270$ K, $p = 1$ kgf/cm^2), equal to 0.522 Q.

Then, the thermal energy of the end reaction products at temperature 1270 K will be equal to 0.642 times the reaction heat of the initial mixture.

The sum is $0.642 + 0.689 = 1.331 > 1.0$. Therefore, the huge efficiency of 0.689 resulting from this naïve calculation, in fact, contradicts conservation of energy. This calculation is absolutely incorrect as we already pointed out.

4. Notes About Potential Practical use of Detonation Cycle

The principally achievable efficiency of detonation-combustion cycle is only slightly larger (by 13% or less) than that of usual closed-volume combustion, so it is rather unlikely that detonation combustion can be used in practice for energy production. It is largely an illusion that, due to the enormous propagation speed of detonation, the burning in detonation combustion is more intense. During actual detonation in tubes, it is the speed of refueling rather than the detonation speed that is the determining parameter. Besides, a closed-volume combustion can be arranged quite fast and complete, especially if using a number of well-known techniques employed in internal combustion engines, such as swirling the mixture or using a pre-combustion chamber that shoots in a torch of flame, etc. Also, detonation needs to be established in a tube in such a way that the kinetic energy of combustion products can be used because only in this case the mixture moves in the same definite direction. Note that if the motion of detonation products is stopped in vain by a collision of detonation wave with a wall, the efficiency becomes exactly equal to that of a constant-volume explosion.

When detonation is done in a tube or a system of tubes, there will be unavoidable considerable losses due to heat absorption through and deceleration of combustion products by the side walls of the tube(s). Therefore, we believe that there are no prospects in searching for detonation-combustion cycles in a chase after a slightly larger theoretical efficiency. At the same time, one should keep in mind, on one hand, various losses unavoidably reducing the efficiency achievable in practice and, on the other hand, a trivial possibility to increase the combustion efficiency by pre-compressing the mixture. It is noteworthy that over the last 20 years, engineers have primarily studied gas turbines with constant-pressure combustion even though their efficiency is lower than that of the explosion turbine (given the same initial pressure).

The decisive factors were the simplicity of implementation and reduction of losses in a continuously operating machine.

5. Use of Detonation in Air-Breathing Jet Engine

Consider a problem of possible continuous (standing) detonation combustion of the fuel in an air-breathing jet engine that moves with a speed approximately equal to the propagation speed of detonation. Fig. 4 shows an approximate schematic.

The air entering from the left at a supersonic speed is carbureted with the fuel entering through tube C. The explosive mixture burns in the detonation wave whose front is denoted by line AB. Combustion products expand in Laval nozzle Λ_2 to the atmospheric pressure. This scheme should be compared to the usual scheme of an air-breathing jet engine, shown in Fig. 5 for the motion at a supersonic speed. The air loses virtually all of the dynamic pressure when its speed decreases from supersonic to subsonic in Laval nozzle Λ_1 and then decreases further in the diffuser. The air is carbureted with fuel at the entrance C or later (carburetor position C') to prevent premature spontaneous ignition during compression. The comparatively slow-moving mixture burns in zone $A - B$, and combustion products expand in Laval nozzle Λ_2, doing work. It is very easy to compare the two schemes (only in principle!) based on understanding the mechanism of combustion in a detonation wave.

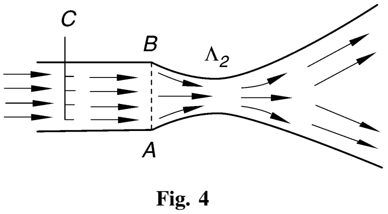

Fig. 4

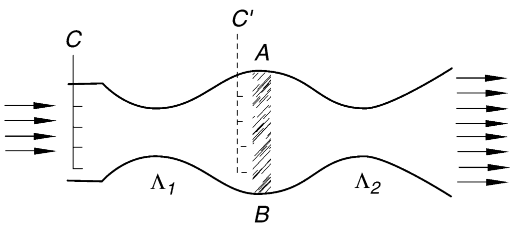

Fig. 5

In terms of this understanding (for details, see our work loc.cit.), detonation combustion proceeds as a matter of fact in two stages (Fig. 6). The first stage is an adiabatic, but not isentropic compression of gas in the shock wave; the propagation speed of the shock wave is equal to the detonation speed, and point I represents the post-compression state in the p–v plane. Under the conditions at point I, a fast chemical reaction begins in the explosive mixture. It is accompanied by heat release and change of state along the line I–D. At the end of the reaction, combustion products are in state D (cf. Fig. 3). Comparing now the detonation combustion with the classical scheme of Fig. 5, we can easily establish that the former (detonation) is accompanied by a greater increase in entropy. Thus, entropy grows irreversibly during the shock wave compression, which happens over a distance of the order of the mean free path of gas molecules. On the contrary, in the Laval nozzle, isentropic compression can in principle be achieved. The entropy growth during the combustion of the moving gas in the process described by segment ID (Fig. 6) also exceeds the entropy growth under combustion of isentropically compressed gas at constant pressure in region AB (Fig. 5) because in the latter process, the heat of the chemical reaction is released on average at a higher temperature. It is obvious that all these entropy losses will result in a greater (in the case of detonation, Fig. 4) thermal energy of the combustion products that are escaping into the atmosphere—which will reduce their speed, the recoil force, and the efficiency of the jet engine.

Note that for our task it was not necessary to consider the mechanism of detonation combustion and the state I of the compressed gas because the classical theory after all fully determines the end state D of the detonation products. Therefore, we could have also obtained our conclusion about the smaller efficiency of detonation in this case by a direct general calculation. We considered this mechanism only to derive the end result quickly and instructively.

We will illustrate the above by a numerical example for a mixture whose thermal characteristics were given in the previous section. Assuming the density of air (mixture) is initially 1.2 kg/m^3, the speed of the detonation wave is

$$D^2 = v_0^2 \frac{p - p_0}{v_0 - v} = RT_0 \frac{15.55 - 1}{1 - 0.6} = 36.4RT_0; \qquad D = 1730\,\mathrm{m/s}$$

The speed of the air-breathing jet engine should also be 1730 m/s. The temperature of gases escaping at the atmospheric pressure is again 1270 K. The Bernoulli equation in the system of coordinates that moves together with the rocket allows us to find the escape velocity u_1:

$$J_0 + D^2/2 = J + u_1^2\big/2$$

$$[k/(k-1)]RT_0 + Q + D^2/2 = [k/(k-1)]RT + u_1^2\big/2$$

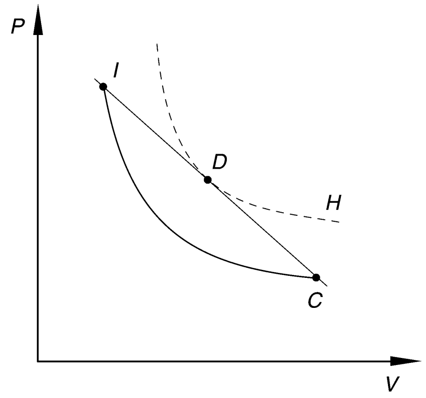

Fig. 6

Substituting $Q = 10500 = 17.5RT_0$, $k = 1.4$, and $T = 1270 = 4.23T_0$, we find

$$3.5RT_0 + 17.5RT_0 + 18.2RT_0 = 3.5 \cdot 4.23RT_0 + u_1^2/2$$

$$u_1^2 = 48.8RT_0; \qquad u_1 = 2005\,\mathrm{m/s}$$

The speed of the combustion products relative to the atmosphere is

$$\Delta u = u - D = 2005 - 1730 = 275\,\mathrm{m/s}$$

At the same time, according to the Bernoulli theorem (energy conservation law), the isentropic compression of the cycle in Fig. 5 results in the following state of the stagnant gas:

$$J_0 + D^2/2 = J; \qquad 3.5RT_0 + 18.2RT_0 = 3.5RT$$

$$T = 6.2T_0; \qquad p = p_0(T/T_0)^{3.5} = 600p_0(!)$$

After the combustion at constant pressure p, the temperature reaches

$$T' = T + 10500/7 = T + 5T_0 = 11.2T_0$$

During the further expansion from 600 (!) kgf/cm^2 to 1 kgf/cm^2, the temperature drops to its final value:

$$T_k = T'/6.2 = 1.81T_0 = 543\,\mathrm{K}$$

Finally, the escape speed of the combustion products is

$$u_1^2 = 65.8RT_0; \qquad u_1 = 2325\,\mathrm{m/s}$$

$$\Delta u = 2325 - 1730 = 595\,\mathrm{m/s}$$

The losses in the detonation cycle decrease by a factor of two the thrust of the jet engine compared to the cycle with isentropic compression and constant-pressure combustion if one considers a rather high rocket speed equal to the propagation speed of detonation.

6. Summary

1. We have considered the question of achievable efficiency of cycles that use detonation combustion. The work which can be performed by the combustion products immediately after the completion of the chemical reaction (which reached 69% of the reaction heat in the numerical example) cannot be used fully. It is necessary to use a fraction of it to sustain the detonation combustion.

2. Still, the efficiency of a cycle that uses detonation combustion without any losses is, in principle, always somewhat larger than that of a cycle that uses closed-volume combustion (in the above numerical example, 35.4 versus 31.3%).

3. Pre-compressing the explosive mixture increases the efficiencies of both detonation combustion and slow combustion, but decreases the difference between the two.

4. The difficulty of carrying out and using the detonation with minimal losses makes the attempts of practical application of detonation combustion to energy production inadvisable.

5. In a supersonic air-breathing jet engine with continuous combustion, detonation combustion results (in absence of losses) in a lower thrust compared to the usual cycle.

Appendix

When we compared detonation with a closed-volume explosion (Section 2), we calculated the state of the explosion products in the simplest way (point E, Fig. 3). As is well-known, in reality after the propagation of flame in a closed volume, different volume elements end up in different states upon combustion (so-called Mache[6] effect). The volume element that has burnt first, afterwards undergoes the adiabatic compression from the initial pressure to the final pressure of the explosion, and its temperature attains the highest value, etc. The explosion temperature that we have found in state E turns out to be only the average value. Obviously, the entropy of this temperature distribution M is less than the entropy of the same mass in state E, considered in Section 3, where the temperature is the same throughout the volume.

This is obvious because distribution M evolves into state E as the result of irreversible leveling out of the temperature of the explosion products. Could the smaller entropy of distribution M lead to a larger achievable efficiency? It turns out that during an ideal process, the end products still have a temperature distribution (though on a different scale) so that the entropy of the end products at a given energy is also less than the entropy of state E' (Fig. 3). Assuming for simplicity constant heat capacity, no dissociation, and no deviations from ideal gas behavior, one can easily show that the gas pressure depends only on gas mass, occupied volume, and the full (or average) energy of all the gas, but does not depend at all on the energy distribution in the gas. In particular, with these assumptions the pressures for state E and for distribution M must be exactly equal to each other. A numerical calculation that takes into account dissociation, actual specific heats, etc. gives

$$\frac{p_M - p_E}{p_E} \simeq -0.01 \text{ to } -0.02$$

i.e., a very small deviation. Moreover, this deviation is negative and so reduces the efficiency, as we will see shortly. Let us go back to the method that Poisson used in 1818 to write down the adiabatic equation long before the concept of entropy was introduced. The equation

$$dE = -pdv$$

is equally valid in an adiabatic process both for the specific energy and specific volume of a small portion of fluid, whose internal temperature can be considered uniform, as well as for the full energy and full volume of explosion products with any temperature distribution. Since a similar equation relates pressure, energy, and volume (for any ideal gas with constant specific heats), the work done during expansion will be also the same for a fluid in state E and the actual distribution M. Therefore, our calculation remains correct to within 1-2%. The same can be said about the temperature distribution, different from M, that arises after detonation combustion and subsequent deceleration of detonation products through collisions of the wave with vessel walls.

The decrease in power that occurs at the onset of detonation in internal combustion engines is due to the increase in heat transfer and other losses that we do not consider here. The attempts of thermodynamic descriptions of this decrease in efficiency are wrong.[7]

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[6] Translation note: See the discussion on p. 148 of W. Jost's textbook "Explosion and Combustion Processes in Gases," McGraw–Hill 1948. Jost makes reference to the paper of Flamm, H. and Mache, E. *Wien. Ber.*, **126**, 9, 1917 in his description of the theory of vessel explosions.

[7] Brown. Chem. Rev., **22**, 27, 1938.

Note Added in Proof

After this article went to press, S.B. Ratner[8] did a calculation of state D for a stoichiometric gasoline-air mixture considering all dissociation reactions and temperature dependence of specific heats, and using the E-S diagram of Hottel et al.[9] for the combustion products of octane (C_8H_{18}) in air. His numerical results differ very slightly from the example in this paper: In state D, the pressure is 17.5 kgf/cm^2, temperature is 2780 K, and specific volume is $0.582v_0$. Upon the expansion to the atmospheric pressure, the temperature drops to 1780 K. The efficiency is 32%. During constant-volume combustion (point E), the pressure reaches 9.6 kgf/cm^2, the temperature is 2620 K, and $v = v_0$. After the work is done, the temperature drops to 1825 K, and the efficiency is 28.6%.

Changing from closed-volume combustion to detonation therefore increases the efficiency of an ideal cycle by 12% instead of 13% as in the numerical example in this paper.

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Received by the Editor on June 15, 1940.

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[8] Ya.B. Zeldovich and S.B. Ratner. *Journal of Experimental and Theoretical Physics*, Vol. 10, No. 12, 1940.

[9] Hottel and Hershey. SAE Journ., **39**, 414, 1936.