# A THERMODYNAMIC ANALYSIS OF THE RATE OF RISE OF PRESSURE IN THE OTTO CYCLE

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Approximately two-thirds of the mechanical horsepower of the nation is developed by internal-combustion motors operating on the Otto cycle. In the ideal cycle (figure 2) the mixture is compressed adiabatically from 1 to 2, and the combustion is supposed to take place instantaneously at constant volume over the path 2-3. The burned gases then expand adiabatically from 3 to 4, at which point the exhaust valve opens and the mixture expands from 4 to 4', leaving within the cylinder that quantity represented by point 5. On the exhaust stroke from 5 to 6 most of the burned mixture is forced out of the engine cylinder, that volume represented by point 6 being retained in the clearance volume. The charge is then drawn in along the intake stroke from 6 to 1, and the cycle is repeated.

#### I. THE NORMAL CYCLE

The actual combustion does not take place instantaneously, but begins at a single point or zone where ignition occurs. Inflammation spreads rapidly throughout the entire mixture, with each succeeding part to be inflamed burning under conditions of higher pressure and temperature than the previous zone. Such a reaction is not a true homogeneous reaction in the sense that the gas is a single homogeneous phase during combustion, but only in the sense that the reaction takes place in a gas phase which is strictly a single phase only before and after combustion and is unaffected by surfaces. Such a reaction has been called "progressive homogeneous" (2). The combustion may be expressed diagrammatically, as in figure 1. Condition A represents that immediately before ignition. B represents the complete inflammation of layer 1 and its expansion compressing the unburned gas ahead of the flame. Condition C represents the inflammation of layer 2, which expands and compresses the burned gases in layer 1 and the unburned gases ahead of the flame. procedure is indicated in a further stage of combustion in D.

If the combustion proceeds orderly in this manner at a moderately low

rate, pressure is equalized throughout the gaseous mixture as the flame advances. The normal combustion Otto cycle is an idealized cycle, assuming this type of normal combustion to take place while the piston is at top dead center. Figure 3 indicates the specific properties of the first and last layers of the mixture to burn in this manner as computed by the thermodynamic chart of Hershey, Eberhardt, and Hottel (13). The expansion and compression of the successive layers of gas burned in such a progressive combustion reaction establish a temperature gradient throughout the burned mixture, as may be computed (13) and as has been measured (14, 22).

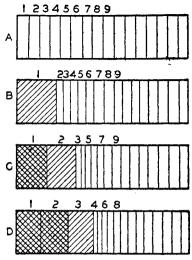


Fig. 1. Normal combustion. A represents the charge before ignition, B the conditions when layer 1 is inflamed, C the conditions when the flame has passed 1 and 2 is inflamed, and D the conditions with a fast burning mixture when pressure is not uniform but is concentrated in the flame front.

The use of the enthalpy—entropy charts takes into consideration changes in heat capacity and equilibrium in the product of combustion. They are considered to give reliable results depending upon the assumption made in their application. For convenience the computations that may be made by the use of the ideal gas equation, ignoring chemical equilibrium, have been outlined in the appendices.

The temperature gradient at the end of normal combustion, assuming adiabatic processes and no mixing, with uniform pressure distribution during combustion with the piston at top dead center, is computed as 1500°F. for ideal gas mixture (see Appendix II(3)), and as 763°F. by means of the thermodynamic equilibrium chart. In each case a compres-

sion pressure of 160 lb. per square inch and a combustion pressure of 760 lb. per square inch absolute were assumed. The relatively large difference in the two methods is due to the fact that variations in heat capacity and dissociation have been accurately computed in the thermodynamic charts and neglected in the simple equations assuming ideal gases. An interesting comparison with experimental data is provided from tests on an engine of 4.4 compression ratio, using 80 per cent of theoretical air (22) in which a temperature gradient of about 600°F. was measured. The computed temperature gradient for this compression ratio, using 85 per cent of the theoretical air according to the thermodynamic chart (13), is 1030°F. When it is considered that 40° of crank revolution was required for com-

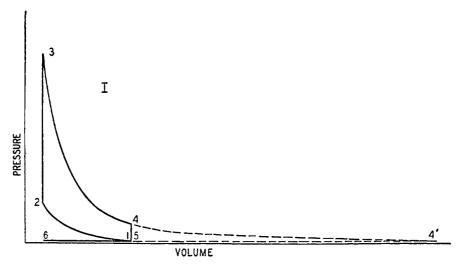


Fig. 2. Pressure-volume diagram of the ideal Otto cycle I

bustion in the engine, as well as that there were other differences, and that it is impossible to measure the temperature of the extreme first and last layers burned, the agreement appears satisfactory.

Insofar as efficiency and work are concerned, the ideal instantaneous combustion Otto cycle and the normal combustion Otto cycle are closely equivalent (13a). This is due to the fact that combustion occurs with the piston at top dead center in each case and with no important thermodynamic irreversibility other than that of the chemical reaction itself. These two cycles are identified as cycle I of figure 2 and cycle II of figure 3, as computed from the thermodynamic charts using 85 per cent of theoretical air (13). The properties of the working fluid at the various points as calculated are given in table 1. The slight differences between cycles I and

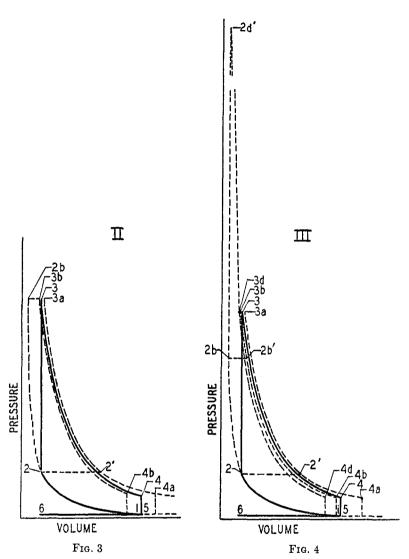


Fig. 3. Pressure-volume diagram of the normal Otto cycle. The solid lines represent average or effective properties, and the broken lines represent specific properties of the first (a) and last (b) parts of the mixture to be inflamed.

Fig. 4. Pressure-volume diagram of a knocking Otto cycle in which one-third of the charge detonates at constant volume. The solid lines represent average or effective properties and the broken lines specific properties of the first (a) and last (b) parts to burn normally with uniform pressure distribution and of the detonating (d) part of the mixture.

TABLE 1

Computed properties of working fluid in adiabatic Otto cycle

Compression ratio = 6

Compression ratio = 0										
POINT	CACTE	DESCRIPTION	A ABSOLUTE TEMPERATURE R.	ABSOLUTE PRESSURE LB. PER SQ. IN.	VOLUME OF GASES PER LB. OF AIR	H RELATIVE ENTHALPY PER LB. OF AIR	RELATIVE INTERNAL  C ENERGY PER LB.  OF AIR	RELATIVE ENTROPY OF PER LB. OF AIR		
1	I, II, III	Begin compression	<b>65</b> 0	14.7	16.8		26.			
$oldsymbol{z}_{\mathtt{b}}$	I, II, III II	End of compression Last to burn at con-	1152	160	2.8	·	138,	0.11.		
$2_{\rm b}$	III	stant P Last to burn at con-	1640	760	About 0.9	1836		0.11.		
-5		stant P	1 <b>52</b> 0	560	1.08	335.	228	0.11.		
3 2'	I II, III	End of combustion First to burn at	4980	<b>7</b> 60	2.8		1585	0.576		
$2_{ m b}^{\prime}$	III	constant <i>P</i> Last to burn at con-	4308	160	11.2	1676		0.633		
$2_{ m d}^{\prime}$	III	${ m stant}\; P \ { m Constant}\; { m volume}$	4600	<b>5</b> 60	3.55	1792		0.564		
<b>2</b> a	-11-	"detonating"  After equalization of	5255	2020	1.08		1675	0.520		
3 <sub>a</sub>	II	First to burn	5475	760	3.08		1840	0.633		
$3_{\rm b}$	II	Last layer to burn	4712		2.53	1836	1455	0.544		
95	II	Average 3a and 3b	5093	1 1	2.8	1000	1647	0.011		
3 <sub>a</sub>	III	First to burn	5430	725	3.25		1825	0.633		
3 <sub>b</sub>	III	Last to burn at con- stant P	4825		2.56		1520	0.564		
$3_d$	III	Constant volume	4020	120	2.50		1520	0.504		
o <sub>u</sub>		"detonating"	4370	725	2.58		1350	0.52		
	III	Average 3 <sub>a</sub> , 3 <sub>b</sub> , 3 <sub>d</sub>	4875	1	2.8		1565	0.02		
4	I	End of expansion	3300	80	16.8		1010	0.576		
4.	II	First to burn	3820	1 .	18.8		1180	0.633		
$4_{ m b}$	II	Last to burn	3060		14.8		940	0.544		
	III	Average 4a and 4b	3440		16.8		1060			
$4_{\mathbf{a}}$	III	First layer normal	3800	80	19.8		1160	0.633		
$4_{ m b}$	III	Last layer normal	3200	80	16.2		980	0.564		
4 <sub>d</sub>	III	Detonating	2835		14.7		870	0.52		
-	III	Average 4 <sub>a</sub> , 4 <sub>b</sub> , 4 <sub>d</sub>	3280		16.9		1003			
4'	I	End of exhaust		14.7	66	610	723			

II indicated in table 1 are due to the inexact but convenient use of arithmetical averages of the properties of the first and last layers of the mixture to burn. As the same procedure was used for the detonating cycle III as for the normal cycle II, these two cycles are comparable in all respects.

In these figures a solid line represents the average properties of the working fluid in the cycle. The dashed lines in figure 2 (cycle I) indicate the specific properties of the fluid at the end of expansion and with the exhaust valve open with the piston at lower dead center. The dashed lines in figure 2 (cycle II) indicate the specific properties of the first and last infinitesimal layers to be inflamed, assuming adiabatic conditions without mixing and uniform pressure distribution during combustion.

### II. THE KNOCKING CYCLE

If the inflammation is accompanied by an extremely high rate of rise of pressure so that the pressure is not uniformly distributed throughout the mixture, as has been indicated in figure 1 D, which shows the layers 4 and 5 immediately ahead of the inflamed layer 3 compressed to a greater degree than the unburned gas toward the right end of the cylinder, a zone of high pressure is built up directly ahead of the flame and within the flame. Under these conditions the inflamed layers of gas at a high pressure expand very rapidly, compressing those layers of gas at low pressure in sequence with a velocity equal to the velocity of a sound wave in the gaseous medium (15). This action establishes a high intensity pressure wave traveling back and forth through the mixture and reflected from the walls of the combustion chamber. The immediate cause of such a pressure wave is the extremely high rate of rise of pressure developed in a part of the mixture and the extremely rapid expansion of this high pressure zone against the low pressure zone within the mixture. Such an expansion takes place with extreme speed and is thermodynamically highly irreversible, in that the work energy lost by the zone of high pressure equals

# $\int P_1 \mathrm{d}V$

while the work done by the zone of high pressure on the zone of low pressure is equal to

# $\int P_2 dV$

Since dV is the same in the two expressions and  $P_1$  is much greater than  $P_2$  at the beginning of the expansion, although equivalent at the end, it is clear that the expansion of the high pressure zone against the low pressure zone is thermodynamically irreversible. However, the pressure immediately ahead of the high pressure zone is locally equal to  $P_1$ , because of the high velocity of expansion and the high rate of rise of pressure. Therefore

the path covered by the high pressure zone during expansion is correctly represented by an adiabatic path corresponding to the  $\int P_1 dV$  above as is the  $\int P_2 dV$  representative of the path for the low pressure zone.

The apparent loss in potential energy accompanying this irreversible expansion is evident in the high velocity intense pressure wave as kinetic energy, the conversion of potential energy into kinetic energy being necessary to accomplish the extremely rapid expansion caused by the high rate of rise of pressure in the high pressure zone.

In fuel-oxygen mixtures the rate of reaction and the rate of rise of pressure in the flame front are so intense that the condition outlined above is obtained in the case of an otherwise normal progressive combustion and results in the detonation wave (9, 26), in which the unburned mixture immediately ahead of the flame front is ignited and inflamed by the intense adiabatic compression, so that the detonation wave is supported by the inflammation which is part of the pressure wave itself.

In fuel-air mixtures the rate of reaction is retarded by the presence of diluent, and the true detonation wave is not ordinarily developed. However, in high-compression engines the compression of the unburned charge ahead of the flame front by the process of normal combustion in which the pressure is uniformly distributed in the manner described frequently brings the unburned charge to such a condition of temperature and pressure that it spontaneously bursts into flame, accompanied by an intensely high rate of rise of pressure due to the extremely rapid inflammation. The effect of this extremely high rate of rise of pressure caused by the autoignition, or "detonation", of the unburned charge results in the same type of spontaneous, thermodynamically irreversible expansion of the high pressure zone against the low pressure zone of gases in the combustion chamber immediately following such autoignition. This results in the intense pressure wave which is similar in most respects to the detonation wave described above, except that it is not accompanied by the simultaneous inflammation of an unburned mixture.

This mechanism of engine detonation has been indicated for many years on the basis of experiments in bombs (32, 7), and has been confirmed by photographic studies of detonating mixtures in the combustion chamber of an engine (25, 23). In these studies (23) normal combustion at 900 R.P.M. required 36° of crank rotation or about 0.0067 second for complete inflammation. Knocking or "detonating" combustion under the same speed and other conditions required a total of only 22° rotation or about 0.0041 second for complete inflammation. The normal combustion of approximately one-half by weight of the mixture required the same time in each case,—about 0.0036 second. But the autoignition of the last half of the charge in the knocking combustion required only about 0.0005 second for

complete inflammation. The photographs (23) clearly indicate that autoignition and inflammation of the last half of the charge during 0.005 second takes place without observable change in the position of the previously burned gases, that is, at substantially constant volume.

In figure 4 is shown cycle III, which represents the normal combustion of two-thirds of the explosive mixture followed by autoignition or detonation of the last third of the mixture, computed by means of the thermodynamic charts (13), assuming 85 per cent of theoretical air and the same compression ratios and initial conditions as for cycles I and II. The normal combustion of the first two-thirds of the mixture was assumed to take place with uniform pressure distribution throughout the charge, and the autoignition or knocking of the last third of the mixture to be inflamed was assumed to take place at constant volume. The entire process is assumed to be adiabatic, and the various zones of gases are assumed to expand or to be compressed without mixing under adiabatic conditions in the same manner as was assumed in computing the normal combustion of cycle II (13) represented in figure 3.

The properties of the working fluid corresponding to the different points in cycle III are included in table 1. It will be noted that the compression of the charge along the path 1-2 is the same for all three cycles. The first infinitesimal layer to be inflamed is ignited under conditions corresponding to point 2 and burned with pressure constant and uniformly distributed throughout the mixture along the path 2-2'. Along this path the enthalpy of the mixture remains constant. Normal combustion proceeds in successive layers compressing the unburned mixture ahead of the flame adiabatically along the path 2-2b. At 2b the last layer is inflamed and burns at constant pressure 2b-3b. In cycle II this completes the entire combustion. But in the knocking cycle III this normal combustion is assumed to continue for only two-thirds of the charge, and upon combustion of the last layer to burn normally along the path 2b-2b', one-third of the charge, at conditions corresponding to 2b, is still uninflamed.

In cycle III the balance of the combustion is assumed to take place at constant volume along the path 2b to 2d'. At the instant of the completion of this constant volume combustion or autoignition of the last third of the charge, that part of the charge which has burned normally is at the pressure represented by the horizontal line 2b-2b', while that part which has detonated is at the pressure 2d'. This large difference in pressure requires that the high pressure zone at the pressure 2d' expand with a high velocity along the adiabatic path 2d'-3d, thereby compressing the previously burned charge for the pressure 2b' to the point 3b for the last layer to be burned normally and to the point 3a for the first layer to be burned. After this expansion the mean effective pressure corresponds to point 3.

This is the pressure which is effective on the piston in doing useful work, as the instantaneous high and low pressures in the high velocity pressure wave are not effective in accomplishing any useful work on the piston.

The computation for this adiabatic irreversible expansion has been made in exactly the same way as was proposed by the authors of the charts (13) for handling the irreversible expansion of the exhaust gases from the combustion chamber through the exhaust valve to atmospheric pressure at the end of the expansion zone. The temperatures and pressures of the various parts of the mixture so computed and listed as table 1 indicate that the maximum temperature in the detonating combustion is found not in that part of the mixture to detonate (point 2d, cycle III) but in the first layer of mixture to be inflamed (point 3a, cycle III). This difference in temperature persists throughout the expansion stroke in the same manner as the temperature gradient in normal combustion cycle II previously discussed.

The pressure developed in the detonating part of the charge is much higher than that effective in any other part of the mixture. In table 1 an absolute pressure of 2020 lb. per square inch is indicated for the detonating part of the charge, as compared with an effective pressure of 725 lb. per square inch absolute for other parts of the charge. It is true that this high pressure in the detonating charge exists only for an extremely short interval of time and that it is not effective in doing work on the piston, although it has been referred to as an effective pressure because it is the motivating force for the high pressure wave which is set up in detonating explosions (25) and is accompanied by enormous acceleration in the pressure—time curve of the detonating portion of the charge.

If the observed time of autoignition at 900 R.P.M. for one-half of the charge (23) be assumed as the time interval for the detonation of one-third of the charge in cycle III, the average rate of rise of pressure during the detonation would be

$$\frac{2020-560}{0.0005}$$
 or 2,920,000 P.S.I. per second

The average rate of rise of pressure for the normal combustion preceding knock may be estimated as

$$\frac{560 - 160}{0.0036}$$
 or 120,000 P.S.I. per second

These figures indicate an average acceleration of the rate of rise of pressure during detonation or knock of about

$$\frac{2,920,000-120,000}{0.0005}$$
 or 5,600,000,000 P.S.I. per second per second

Maximum acceleration of the pressure-time curve during detonation at speeds of 2000 R.P.M. might be 10 to 500 times this estimated average. Such forces exerted on the head and piston of the engine cause an accelerated deflection of engine parts, resulting in a maximum deflection greater than would be caused by the application of the same maximum pressure if the maximum pressure had been attained more gradually (16).

These enormous forces developed by the detonating part of the charge have an intense local action on the surrounding part of the combustion chamber and may be the true cause for the destruction of part of alloyed pistons when operated under severe detonating conditions. The apparent fusion of such pistons in the detonating zone cannot be due to the temperature developed therein, as this is actually less than that developed in the first layer to burn (compare point 2d and point 3a of cycle III in table 1).

The computed average effective pressure at the end of combustion for cycle III is 725 lb. per square inch, as compared with 760 lb. per square

TABLE 2

Computed effect of knocking on power and efficiency in adiabatic Otto cycle

Compression ratio = 6

	NORMAL	KNOCKING
Cycle	II	III
Work done = $(U_3 - U_4) - (U_2 - U_1)$ averages, in  B. t. u	475	450
Calculated efficiency based on 19,240 × 0.0749 B. t. u. for net heat combustion of fuel per pound of air, in per cent  Mean effective pressure, in pounds per square inch	32.9 182	31.0 172

inch for the normal cycle II. This loss in effective pressure chargeable to the thermodynamic irreversibilities involved in the mass equalization of pressure following combustion results in a loss of about 5.5 per cent in net work, efficiency, and mean effective pressure of the cycle, as indicated in table 2.

The application of the ideal gas laws to the computation of such a knocking cycle (11) is indicated in Appendix II(4), with an indicated average pressure for the end of combustion (point 3) of 730 lb. per square inch as compared with 725 lb. per square inch for cycle III computed from the charts (13).

Since the power developed by such cycles depends entirely upon the increase in pressure accompanying combustion, it is interesting to note that the loss in work and efficiency due to knocking is proportional to the loss in effective rise in pressure upon combustion. This loss in rise of pressure is computed as 5 per cent, using the ideal gas equation as in

Appendix II, and 5.83 per cent as computed by the thermodynamic charts (13).

An experimental confirmation of the loss in power due to detonation as computed upon these assumptions is provided by test data taken on a variable compression N.A.C.A. Universal test engine and reported some

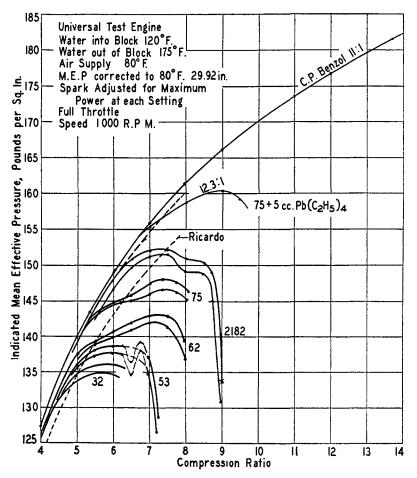


Fig. 5. The effect of compression ratio on the power (mean effective pressure) developed by different fuels in the N.A.C.A. Universal test engine.

years ago (3). Figure 5, reproduced herein, is a plot of the mean effective pressure as a function of compression ratio as observed for different fuels. Fuel 2182 developed incipient detonation at a compression ratio of about 6.

The increase in compression ratio beyond that at which incipient detona-

tion develops, sufficient to cause detonation of one-third of the mixture as assumed for cycle III, may be computed by equation 17 as derived in Appendix I(4), as has been done in Appendix II(4). As indicated therein, an increase in compression ratio of about 33 per cent based on a compression ratio of 6.25 for incipient detonation, would be sufficient to cause the last third of the charge to detonate.

At a compression ratio of 8, which is an increase of 33 per cent over a compression ratio of 6, fuel 2182 developed a mean effective pressure of about 151 lb. per square inch, compared with a mean effective pressure of about 161 lb. per square inch for benzene, which does not detonate under these conditions. The mean effective pressure developed by benzene is about 1 per cent greater than that developed by fuel 2182 at lower compression ratios where neither fuel knocked. Making this adjustment for the different fuels, as indicated by the dashed extension of the curve for fuel 2182 in figure 5, the loss in mean effective pressure caused by detonation of fuel 2182 at a compression ratio of 8 is about 9 lb., as compared with a mean effective pressure of 160 lb. for non-detonating conditions. This corresponds to a loss of 5.6 per cent for the computed detonation of one-third of the charge. This is in excellent agreement with the 5.5 per cent computed for an idealized cycle by the thermodynamic charts (13) as given in table 2.

Similar calculations for fuel 62, which showed incipient detonation at a compression ratio of 4.7, indicates a loss in mean effective pressure of 5.3 per cent due to detonation at a compression ratio of 6.3, which is an increase of 33 per cent over that compression ratio required for incipient knock. Similarly fuel 75, showing incipient detonation at a compression ratio of about 5.3, indicates a loss in mean effective pressure of 5.1 per cent, owing to detonation at a compression ratio of 7.1.

These test results on different fuels of different knock ratings, showing approximately the same relative loss in mean effective pressure on detonation as computations based on adiabatic cycles, indicate that the loss in power and efficiency due to detonation may have a thermodynamic explanation in the loss of availability in the thermodynamic irreversibility of pressure equalization after detonation independent of any increased loss of heat by heat transfer from the gases to the jacket. The conversion of heat into work is a "second law" problem and is greatly reduced by thermodynamic irreversibility.

If the kinetic energy evident in the intense pressure wave caused by detonation were immediately converted to heat energy by absorption within the gaseous mixture, it might be expected that there would be no loss in power to the detonation. But the photographs of detonating combustion in engines show that these pressure waves persist for some

time (25), and it would appear more reasonable to assume that they are damped by the absorption of their energy in the walls of the combustion chamber rather than by the mixture itself. The computation based on an adiabatic cycle confirms this interpretation. As correctly stated by Rassweiler and Withrow (24), this loss in power and efficiency "must be accounted for by differences between knocking and non-knocking explosions other than a temperature difference of the gases", as they had observed that the temperature of the gases was actually lower in knocking combustion than in normal combustion. This difference is also evident in the computed cycles III and II as indicated in table 1. Increased heat transfer due to the pressure waves following detonation may be an unnecessary assumption.

These pressure waves of high intensity developed by detonation must not be confused with the vibrations which are frequently observed in normal burning mixtures (9, 15) even if such vibrations take on the properties of a pressure wave (26), owing to the acceleration of the flame (9) and the accompanying intensification of the vibrations as it passes through the flame front. These vibrations are apparently caused by oscillations in the igniting spark (26); when suppressed or eliminated by proper control of the spark no shock wave was developed upon autoignition in a cylindrical bomb (26).

These pressure waves, combined with a high rate of rise of pressure in the last part of the mixture to burn, may be the cause of roughness in engines, as in bomb experiments this combination was found to develop sound and vibrations in a similar manner (26).

#### III. ROUGHNESS

Intermediate in outward characteristics to knocking and normal combustion is another phenomenon characterized as "roughness", which is caused by high rates of rise of pressure or, more correctly, by high accelerations in the rate of rise of pressure. Janeway (16, 17) has analyzed combustion as related to roughness and has set forth the quantitative characteristics of two normal explosions (table 3), each developing the same maximum pressure with uniform pressure distribution throughout the combustion period, but one of smooth combustion characteristics and the other rough.

If the combustion chamber and location of the spark plug are so designed that the increase in volume of the flame with length of travel from the source of ignition is large during the early part of combustion and reduced during the later stages of combustion, the rate of rise of pressure is more nearly uniform with greatly reduced maximum acceleration (16, 17). This makes for a smooth combustion and a retarded rate of rise of pressure

during the combustion of the last part of the charge. This design is equivalent to igniting the mixture in a conical chamber by placing the spark plug centrally a short distance in from the base. The larger volume of the charge is then inflamed before it has been highly compressed by the expansion of previously inflamed mixture, and a much smaller part is burned under conditions which tend toward a high rate of rise of pressure. This tends to increase the acceleration in the rate of rise of pressure during the early part of combustion and to reduce the high acceleration which would otherwise occur in the last part of the mixture to be inflamed. The result is a smooth combustion which is otherwise difficult to obtain in high-compression motors.

TABLE 3
Quantitative comparison of smooth and rough engine (17)

	SMOOTE	ROUGH	RELA- TIVE
Maximum rate of rise			
Pressure, in pounds per square inch per			
second	162,300	34,000	2.18
Restoring force, in pounds per square inch			
per second	188,370	465,000	2.47
Maximum acceleration in rise			
Pressure, in pounds per square inch per			
second per second	93,000,000	567,000,000	6.1
Restoring force, in pounds per square inch			
per second per second	149,000,000	605,000,000	4.05
Relative kinetic energy of deflecting mass,			
$(2.47)^2\dots\dots\dots\dots\dots\dots$			6.10
Maximum restoring force, in pounds per			
square inch	439	543.7	
Maximum pressure, in pounds per square inch.	410	410	
Shock factor,* per cent	7.07	32.6	4.6

<sup>\* (</sup>Maximum restoring force - maximum pressure - 1)

Maximum pressure

Roughness may result from a high acceleration of the rate of rise of pressure from any cause, and should not be considered simply a mild form of detonation, which apparently always involves autoignition. The cause of roughness may be a distortion of the engine parts (16, 17), similar to but much less severe than that accompanying detonation, which sets up a vibration, or it may be caused by a transverse vibration of the crankcase which passes through a cycle in the same time as the periodic force which produces it, thereby increasing in amplitude from cycle to cycle until the damping forces become equal to the exciting force (12).

### IV. THE RATE OF RISE OF PRESSURE

In order to control roughness, it has been found necessary to limit the maximum acceleration in the time rate of rise of pressure of the combustion. The rate of rise of pressure in the combustion is also a major factor in the control of detonation.

Combustion in the engine (23, 24) is, in all respects so far investigated, similar to the combustion of gaseous mixtures in bombs of constant volume (15, 26). The high degree of turbulence present in high speed engines and absent in bombs serves to increase greatly the speed of inflammation in normal combustion without appreciable change in the mechanism of combustion. This indicates that the reaction is heterogeneous in nature, that is, involving gases in more than one phase at one instant, and that the mechanism of the spread of flame through the mixture involves the transfer of heat or of material substance from inflamed gases to uninflamed gases ahead of the flame.

The results of computations based on the ideal gas laws are qualitatively correct in analyzing the Otto cycle and may also be used to indicate the effect of some factors controlling the rate of rise of pressure during combustion. By this procedure (4), which is briefly summarized in Appendix I(5), it may be shown (equation 20) that the rate of rise of pressure varies directly as some power of the pressure at which the gas is ignited.

The effect of temperature is more complicated but it has been shown (4, 21) that there is a real positive critical initial temperature at which the explosion develops its maximum rate of rise of pressure. This is true whether this critical initial temperature is determined under conditions of constant initial pressure, as is the case when the temperature of the mixture in the intake manifold is varied at constant throttle and speed, or under conditions of constant density, as is the case when the mixture temperature is varied after a positive displacement supercharger or after being confined within the cylinder. But the critical temperature is not the same under these different conditions (21).

## V. FUEL CHARACTERISTICS

Autoignition develops a very high rate of rise of pressure with loss of available work energy and is by its nature a different reaction from normal combustion. It has been indicated (7) that the tendency of a fuel to knock in an engine may be estimated as varying directly with its rate of rise of pressure upon normal combustion and inversely with its ignition temperature. The rate of rise of pressure is directly proportional to the rate of reaction, which is also related to the "ignition lag" (28), so that perhaps all of us are really talking about the same thing but using different language. In any case, it appears that both factors must be considered in

autoignition, although only the rate of reaction need be considered in the case of normal combustion and the detonation wave.

In actual engine operation it is frequently observed that cracked petroleum fuels of an unsaturated and aromatic character are apparently depreciated in antiknock quality as compared with that which would be expected from laboratory tests. It has also been observed that supercharged engines do not so depreciate these fuels. It has been shown (21) that a supercharged engine is operating above the critical initial temperature for maximum rate of rise of pressure, while the normal engine is usually operating below. If the knocking tendency of a fuel is a function of autoignition temperature and rate of rise of pressure (or reaction), the knocking tendency would be increased more noticeably by an increase in temperature in the normal engine, which is below the critical initial temperature, than by an increase in temperature in the supercharged engine, which would tend to decrease the rate of rise of pressure and thereby tend to compensate for the other effects of temperature in stimulating autoignition. These observations would be particularly applicable to aromatic fuels, because of their high autoignition temperature (19).

In at least one case (10) it was found that engine detonation could be eliminated by increasing the inlet temperature when operating at high temperatures, which would be expected if the operation were conducted at a temperature above the critical initial temperature and with a fuel of high autoignition temperature.

## VI. SUMMARY

The thermodynamic approach to combustion and the rate of rise of pressure in the Otto cycle are fruitful in analyzing the effect of different conditions upon the operation of the cycle. It is suggested that the thermodynamic method is an important tool in explaining and analyzing known characteristics such as "engine knock", roughness, and the effect of supercharging on the relative knock ratings of different types of fuels, and also a means of predicting characteristics of such combustion cycles as in the case of the critical initial temperature giving maximum rate of rise of pressure.

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## APPENDIX I

#### 1. THE INCREASE IN PRESSURE ON COMBUSTION

Assume an ideal gas with constant specific heats to which heat is added equivalent to combustion.

 $V_A$  = the constant volume of the combustion chamber,

 $V_1$  = the volume of a portion of the mixture before combustion,

 $V_2$  = the volume of this portion after combustion,

Q = the heat liberated by combustion of unit volume of mixture,

 $QV_1$  = the quantity of heat available to  $V_1$  liberated by combustion of  $V_1$ ,

$$QV_1 = \Delta U_1 + W \tag{1}$$

 $\Delta U_1$  = the increase in energy content of the portion of mixture burned, evident in increased temperature,

W =the work done by  $V_1$  on  $V_A - V_1$  due to expansion of  $V_1$  to  $V_2$ ,

$$\Delta U_1 = \frac{P_2 V_2 - P_1 V_1}{K - 1} = (T_2 - T_1) C_v \tag{2}$$

$$W = \frac{P_2(V_A - V_2) - P_1(V_A - V_1)}{K - 1} \tag{3}$$

 $K = C_p/C_v = \text{ratio of specific heat at constant pressure to that at constant volume,}$ 

$$QV_1 = \frac{(P_2 - P_1)V_A}{K - 1} = \frac{V_A \Delta P}{K - 1} = \frac{V_A \Delta P C_v}{R} = \frac{T_A \Delta P C_v}{P_A}$$
(4)

$$\Delta P = \frac{QV_1 P_A}{C_v T_A} = \frac{QV_1 R}{C_v V_a} = \frac{QV_1 Rr}{C_v V_0}$$
 (4a)

where r= the compression ratio  $\frac{V_A}{V_0}$  and  $V_0=$  the volume of the charge prior to compression.

The increase in pressure  $(\Delta P)$  is directly proportional to the portion burned  $(V_1)$  and the initial pressure  $(P_A)$  and inversely proportional to the heat capacity  $(C_v)$  and the original or initial temperature  $(T_A)$ . For constant intake conditions  $(V_0)$ , the increase in pressure  $(\Delta P)$  upon combustion varies directly as the fraction burned and the compression ratio (r) and inversely as the heat capacity  $(C_v)$ .

2. THE SPECIFIC VOLUME OF A SMALL UNIT MASS OF THE CHARGE (AS REPRESENTED BY AN INDIVIDUAL LAYER IN FIGURE 1) IN NORMAL COMBUSTION

Considering the combustion of successive infinitesimal layers with uniform pressure distribution as in normal combustion,

 $V_0$  = the original volume of small unit mass of the charge,

V<sub>c</sub> = the volume of such mass after being compressed adiabatically by the burning of other portions, and at which it is inflamed,

 $V_e$  = the volume to which such mass expands at constant pressure during inflammation and combustion, and

 $V_f$  = the final volume of such mass after further adiabatic compression by the burning of succeeding portions, the whole at  $P_f$ .

In the first step of adiabatic compression of unburned gas by previous combustion of other parts

$$V_c = \left(\frac{P_0}{P_c}\right)^{\frac{1}{K}} V_0 \tag{5}$$

In the second step of combustion at constant pressure

$$QV_0 = C_p(T_2 - T_1) = \frac{P_c(V_o - V_c)K}{K - 1}$$
 (6a)

From which

$$V_{\bullet} = \frac{Q(K-1)V_0}{KP} + V_c \tag{6}$$

In the third step of adiabatic compression of the burned gas by later combustion of other parts

$$V_f = \left(\frac{P_c}{P_f}\right)^{\frac{1}{K}} V_{\bullet} \tag{7}$$

Substituting equation 5 in equation 6 and the result in equation 7 and rearranging

$$V_f = \frac{(P_c)^{\frac{1}{K}-1} Q(K-1) V_0}{(P_f)^{\frac{1}{K}} K} + \left(\frac{P_0}{P_f}\right)^{\frac{1}{K}} (V_0)$$
 (8)

#### 3. THE PRESSURE DEVELOPED IN THE MIXTURE ACCOMPANYING DETONATION

If combustion of any part takes place with extreme speed so that pressure is not distributed, that portion so burning or "detonating" may be assumed to burn under conditions of constant volume.  $P_d$  = the pressure developed by "detonation" of that part of the charge burning at constant volume.

From equation 4, remembering that  $V_c$  now equals total volume to burn at constant volume and that all of this volume does so burn  $(V_1 = V_A)$ 

$$QV_{0} = \frac{(P_{d} - P_{c})V_{c}}{K - 1} \quad \text{and} \quad Q = \frac{P_{f} - P_{0}}{K - 1} \frac{V_{0}}{V_{0}}$$

$$P_{d} = \left(\frac{Q(K - 1)V_{0}}{V_{c}}\right) + P_{c} = \left(\frac{(P_{f} - P_{0})V_{0}}{V_{c}}\right) + P_{c} \quad (9)$$

$$T_{d} = \left(\frac{P_{d}}{P_{c}}\right)T_{c} = \frac{(P_{f} - P_{0})V_{0}T_{c}}{P_{c}V_{c}} + T_{c} \quad (10)$$

Consider that part of the charge burns normally with pressure uniformly distributed, followed by constant volume combustion without uniform pressure distribution, that is, "detonation" of the last part, and that the pressure is equalized after combustion, rather than during combustion, by adiabatic compression and expansion.

 $P_x$  = final pressure after equalization after "detonation,"

 $V_x$  = final volume of unit mass after such combustion,

 $V_{xn}$  = final volume of unit mass that burns normally,

 $V_{xd}$  = final volume of unit mass that "detonates," and

 $P_f$  = final pressure resulting from normal combustion as before.

Since the total volume of the entire charge remains constant

$$\sum V_{xn} + \sum V_{xd} = \sum V_0$$

Since the quantity burned in normal combustion is proportional to the increase in pressure (equation 4),

$$\sum_{P_0}^{P_c} V_{xn} + V_{xd}(P_f - P_c) = V_0(P_f - P_0)$$
 (11)

From equation 8

$$\sum_{P_0}^{P_c} V_{xn} = \int_{P_0}^{P_c} \left[ P^{\frac{1-K}{K}} \frac{(P_f - P_0)V_0}{K(P_x)^{\frac{1}{K}}} + \left( \frac{P_0}{P_x} \right)^{\frac{1}{K}} V_0 \right] dP$$

$$= \frac{(P_f - P_0)V_0 \left( P_c^{\frac{1}{K}} - P_0^{\frac{1}{K}} \right)}{P_x^{\frac{1}{K}}} + \left( \frac{P_0}{P_x} \right)^{\frac{1}{K}} V_0 (P_c - P_0)$$

$$V_{xd} = \left( \frac{P_d}{P_x} \right)^{\frac{1}{K}} V_c \qquad V_c = \left( \frac{P_0}{P_c} \right)^{\frac{1}{K}} V_0$$
(12)

and equation 9 gives

$$V_{xd} = \left[ \frac{(P_f - P_0) \left( \frac{P_c}{P_0} \right)^{\frac{1}{K}} + P_c}{P_x} \right]^{\frac{1}{K}} \left( \frac{P_0}{P_c} \right)^{\frac{1}{K}} V_0$$

$$= \left[ (P_f - P_0) \left( \frac{P_0}{P_c} \right)^{1 - \frac{1}{K}} + P_0 \right]^{\frac{1}{K}} \left( \frac{1}{P_x} \right)^{\frac{1}{K}} V_0$$
(13)

Substituting equations 12 and 13 in equation 11, cancelling  $V_0$ , and solving for

$$P_{x}^{\frac{1}{K}} = P_{c}^{\frac{1}{K}} - \frac{\left\{P_{0}^{\frac{1}{K}} - \left[(P_{f} - P_{0})\left(\frac{P_{0}}{P_{c}}\right)^{1 - \frac{1}{K}} + P_{0}\right]^{\frac{1}{K}}\right\}(P_{f} - P_{c})}{P_{f} - P_{0}}$$
(14)

$$P_{x}^{\frac{1}{K}} = \left[ \left( \frac{P_{c}}{P_{0}} \right)^{\frac{1}{K}} - \frac{1 - \left[ \left( \frac{P_{f}}{P_{0}} - 1 \right) \left( \frac{P_{0}}{P_{c}} \right)^{\frac{K-1}{K}} + 1 \right]^{\frac{1}{K}}}{\frac{P_{f}}{P_{0}} - 1} \left( \frac{P_{f}}{P_{0}} \frac{P_{c}}{P_{0}} \right) \right]_{P_{0}^{\frac{1}{K}}}^{\frac{1}{K}}$$
(14a)

#### 4. THE EFFECT OF COMPRESSION RATIO ON THE QUANTITY OF CHARGE DETONATING

If an engine is operated at such compression ratio as to be at the limit of normal combustion, that is, so that any higher compression would result in incipient detonation, the compression ratio at which any degree of knock will occur or the degree of knock for any other compression ratio may be estimated by the following equations: From equation 4a

$$\Delta P = \frac{xRr}{C_v V_0}$$

where x = the fractional part of charge burned and r = compression ratio  $\frac{V_0}{V_A}$ .

The pressure reached on completion of normal combustion of x part of the mixture

$$P_a + \Delta P = P_0(r)^K + \frac{xRr}{C_* V_0}$$
 (15)

For the same intake conditions with the same mixture to obtain the same pressure at end of normal combustion

$$P_0(r_1)^K + \frac{x_1 R r_1}{C_v V_0} = P_0(r_2)^K + \frac{x_2 R r_2}{C_v V_0}$$
 (16)

For the same pressure of combustion of the last layer to burn normally

$$P_b = P_0(r_2)^K + \frac{\Delta P}{r_1} (x_2 r_2)$$
 (17)

where  $P_b$  = absolute pressure of the last part to burn normally and  $P_0$  = absolute intake pressure.

If chemical equilibrium be assumed for the products of combustion, similar calculations may be made by use of the thermodynamic charts (13), without assuming ideal gases. In computing the effects of detonation as indicated by these equations, the results are similar by both methods.

5. THE RATE OF RISE OF PRESSURE ON COMBUSTION AS INFLUENCED BY CONDITIONS AND PROPERTIES OF THE MIXTURE

Considering the ideal combustion at constant volume and writing equation 4 in the differential form, and dividing by "dt", the time rate of rise of pressure  $\left(\frac{dP}{dt}\right)$ ,

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \frac{P}{TC_v} \left( \frac{\mathrm{d}Q}{\mathrm{d}t} \right) = \frac{Phk}{TC_v} \tag{18}$$

where  $C_v$  = heat capacity of products of combustion per unit of mixture,

t = time,

h = heat of combustion per unit of mixture, and

k = specific reaction velocity and number of units reacting per unit of mixture per unit of time.

It has been shown (4) that, even in this ideal homogeneous reaction, k has a maximum value for any particular pressure at some finite positive temperature when the order of the reaction is greater than 1. This was demonstrated theoretically on the basis of the well-known effects of temperature and density upon the velocity of gaseous reaction, which lead to the following equation:

$$k = C \left(\frac{P}{T}\right)^{a-1} (e)^{-\frac{B}{T}} \tag{19}$$

where a = the order of the reaction,

B = a constant representing the "energy of activation," and

C = a constant of integration,

from which it may be shown that for any given pressure (P), k has a maximum value when  $T = \frac{B}{a-1}$ .

Thus the well-known fact that the rate of flame travel (32), as well as the rate of rise of pressure (4, 21), may be decreased by an increase in initial temperature may be explained on the basis of the well-known effect of temperature and density upon gaseous reactions.

Combining equation 19 with 18

$$\frac{\mathrm{d}P}{\mathrm{d}t} = C \frac{h}{C_r} \left(\frac{P}{T}\right)^a (e)^{-\frac{B}{T}} \tag{20}$$

By means of this equation it has been shown (4) that there is a real positive value for the initial temperature (T) which will give the maximum rate of rise of pressure upon explosion of an explosive mixture for any given constant initial pressure, P, and if the order of the reaction, a, is greater than 1, the same statement applies to mixtures which may be ignited under conditions of constant initial density.

Similar relationships leading to exactly the same conclusions can be derived by a more complicated procedure, assuming normal combustion or progressive inflammation by a self-propagating flame.

These conclusions have been verified by experimental work in bombs (4, 21). Furthermore, the effect of heat capacity of the products of combustion and of their change with temperature upon the relative value of the initial temperature giving maximum rate of rise of pressure, has also been confirmed experimentally (21) in bombs. The general conclusions regarding the "critical initial temperature" giving maximum rate of rise of pressure have also been confirmed by tests conducted in normal and supercharged engines (21).

It is therefore indicated that the same thermodynamic or macroscopic approach may be used with satisfactory results in problems involving rates as well as those supposed to be at equilibrium.

# APPENDIX II

NUMERICAL CALCULATIONS USING THESE EQUATIONS DERIVED ON THE ASSUMPTION OF

IDEAL GASES

If K = 1.3,  $P_1 = 160$ ,  $P_2 = 760$ .

(1) Compute Q (B.t.u. per cubic foot at  $P_1T_1$ ): by equation 4, since  $V_1 = V_A$ 

$$Q = \frac{P_2 - P_1}{K - 1} = \frac{(760 - 160)144}{(778)(0.3)} = 370 \text{ B.t.u.}$$

(2) Calculate the ratio of the final volume of the last portion to burn to its initial volume: from equation 4

$$Q(K-1) = P_f - P_0$$

and  $P_c = P_f$ . Equation 8 becomes

$$V_{fL} = \frac{(P_f - P_0)V_0}{P_f K} + \left(\frac{P_0}{P_f}\right)^{\frac{1}{K}} V_0$$

$$\frac{V_f}{V_0} = \frac{600}{760 \times 1.3} + \left(\frac{160}{760}\right)^{\frac{1}{1.3}} = 0.608 + 0.307 = 0.915$$

(3) Calculate the ratio of the final volume of the first portion to burn to its initial volume. When

$$P_{o} = P_{o}$$

$$V_{fI} = \frac{(P_{f} - P_{o})V_{o}}{K(P_{o})} \left(\frac{P_{o}}{P_{f}}\right)^{\frac{1}{K}} + \left(\frac{P_{o}}{P_{f}}\right)^{\frac{1}{K}} V_{o} = \left(\frac{P_{o}}{P_{f}}\right)^{\frac{1}{K}} V_{o} \left[\frac{(P_{f} - P_{o})}{KP_{o}} + 1\right]$$

$$\frac{V_{f}}{V_{o_{I}}} = \left(\frac{160}{760}\right)^{\frac{1}{1.3}} \left[\frac{600}{160.13} + 1\right] = 0.307[3.88] = 1.19$$

Since this is an ideal gas and the initial temperature  $T_0$  was the same for all parts of the mixture and  $V_0$  was likewise the same, it follows that

$$T_{f_I} = T_0 \times \frac{P_f}{P_0} \times \left(\frac{V_f}{V_0}\right)_I$$

If  $T_0 = 1150$ °R.,  $T_{fI} = 6500$ °R.,  $T_{fL} = 500$ °R.

(4) Assuming that the last third of the charge burned were to "detonate" and that the quantity of charge burned normally is directly proportional to the increase in pressure in normal combustion, the final pressure after equalization may be computed by equation 14 or 14a derived on the assumption that the working substance is an ideal gas.

$$P_{x}^{\frac{1}{1.3}} = \left[ \left( \frac{560}{160} \right)^{\frac{1}{1.3}} - \frac{1 - \left[ \left( \frac{760}{160} - 1 \right) \left( \frac{160}{560} \right)^{\frac{0.3}{1.3}} + 1 \right]^{\frac{1}{1.3}}}{\frac{760}{160} - 1} \left( \frac{760}{160} - \frac{560}{160} \right) \right] 160^{\frac{1}{1.3}}$$

$$= \left[ 2.621 - \frac{1 - (3.75 \times 0.75 + 1)}{3.75}^{\frac{1}{1.3}} (4.75 - 3.5) \right] 160^{\frac{1}{1.3}}$$

$$= \left[ 2.621 - \frac{1 - 2.797}{3.75} \cdot 1.25 = 3.22 \right] 160^{\frac{1}{1.3}}$$

$$= 159.5$$

This represents a loss of 30 lb. out of 600 lb. pressure rise, or 5 per cent.

(5) Compute the compression ratio  $(r_2)$  that would cause the last third of the charge to detonate if the compression ratio of  $r_1$  is just insufficient to cause incipient detonation.

From equation 4

 $P_{\pi} = 730$ 

$$Q(K-1) = (P_h - P_1)$$

For adiabatic compression

$$\frac{P_1}{P_0} = \left(\frac{V_0}{V_1}\right)^K = (r_1)^K$$

For incipient knock

$$Q(K-1) = P_b - P_0(r_1)^K$$

From which  $r_1$  may be determined by substituting the numerical values

$$\frac{370 \times 778}{144} (0.3) = 760 - 14.7 (r_1)^{1.3}$$

$$r_1 = 6.25$$

Substituting the numerical values in equation 17

$$760 = 14.7 (r_2)^{1.3} + \frac{600}{6.25} \left(\frac{2}{3} r_2\right)$$

$$r_2 = 8.3$$

This corresponds to an increase in compression ratio of 33 per cent at 6.25 ratio to cause the last third of the charge to detonate as referred to the compression ratio just short of incipient detonation.