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THE KNOCK SYNDROME -- ITS CURES AND ITS VICTIMS

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ABSTRACT

The problem of knock is traced back to the earliest scientific paper on combustion in premixed gases written by Mallard and Le Chatelier. The pioneering contributions of Ricardo, Kettering and Semenov are then put in proper perspective. Upon the recognition of the fact that this phenomenon has been, and still is, imposing the major technological constraint upon the automotive and oil industries, its various cures are reviewed. Essential features of combustion instability leading to its onset are then exposed, and the methodology is outlined for a rational attack upon the problem it poses.

KNOCK IS AN UNDESIRABLE MODE of combustion that originates spontaneously and sporadically in the engine, producing sharp pressure pulses associated with a vibratory movement of the charge and the characteristic sound effect from which the phenomenon derives its name. It impairs the power output of the engine by deteriorating the torque and by exerting structural damage. As demonstrated by the evolution of automotive engineering, it imposes thereby the major technological constraint upon the automotive and oil industries.

The characteristic features of knock have been pointed out in the first scientific paper on the propagation of combustion in an enclosure filled with a gas mixture, presented by Mallard and Le Chatelier in 1883 (1)*. Studies of the phenomenon as a symptom of the internal combustion engine date back to Nernst (2), Clerk (3), and their contemporaries.

Ever since then, knock became the subject of intensive studies. The most revealing accounts of them include those of Clark (4), Withrow and Rassweiler (5,6), Draper (7), Miller (8), Boyd (9), Sturgis (10) Kirsch and Quinn (11), and Maly and Ziegler (12). The tremendous effort made in this respect has been duly reflected, of course, in books on combustion and engines. Of special significance are those of Ricardo (13), Jost (14), Lewis and von Elbe (15), Lichty (16), Obert (17), Taylor (18), and, in particular, the text of Sokolik (19) devoted entirely to knock and its related subjects of self-ignition, flame propagation and detonation. There have been also a number of international technical meetings devoted to the problem of knock. The two best known were the colloquium organized by Starkman, Clarke and Myers for the Ninth Symposium on Combustion (20) at Cornell, and the International Symposium organized by Volkeswagen A.G. Research Division in Wolfsburg (21).

To give justice to such a vast subject in a single paper is certainly outside the realm of possibility. The purpose of this exposition is then just to bring to the fore those aspects that, in the opinion of the author, have not been treated with the care and attention they deserve, at a concomitant exclusion of those that have been attentively studied. Thus left out completely are such essential aspects as the chemical kinetic mechanism of the combustion reactions leading to knock, in particular the processes of "cool flames" and their biproducts, such as formaldehyde, acetaldehyde, and hydroperoxide. This does not preclude, of course, either the importance or the relevance of studies currently conducted in this field. Moreover, in view of the prominent role of the syndrome, the exposition is based upon the premise that it is sufficiently well known to dispense completely with an account of its symptoms, and start with a critical assessment of the cures.

*Numbers in parentheses designate references at end of paper.

Salient thermochemical and gasdynamic aspects of knock are then presented and its stochastic nature is revealed, as appropriate for a sporadic and spontaneous process. Thereupon, implications of these concepts, leading to the elimination of the syndrome, are described. Finally, its victims are pointed out. The arguments brought up in this connection are based on the realization of the fallacy of the following universally adopted train of thought that underlies the development of practically all the combustion systems used today for propulsion or power generation: since the natural form of combustion is a flame, the operation of such systems must be based on the use of a solitary flame. The exact meaning of this statement should become evident from what follows.

CURES

Right from the outset it has been realized that, in order to maximize the fuel economy and optimize the performance of internal combustion engines, it is mandatory to operate them at a sufficiently high compression ratio - a goal critically impeded by the onset of knock. This is essentially the premise upon which the development of all the cures to treat this problem has been based. Moreover, as a consequence of the grave importance of the knock syndrome to the evolution of automotive technology, the cures had to be devised before the cause was known - a typical situation in a fast growing engineering enterprise.

Fundamentally, there are three types of cures, each concerned with a different modus operandi and associated with the name of its major contributor: Sir Harry R. Ricardo, Charles F. Kettering, and Nikolai Nikolaevich Semenov.

Ricardo, ably assisted by J.F. Alcock and advised by A.D. Walsh, sought to develop mechanical means in the design of the combustion chamber. His efforts led to the evolution of various geometrical configurations, exemplified by the well known squish-head engine. Although definitely helpful, this method of approaches turned out to be inadequate for a satisfactory solution of the problem.

Kettering, in association with T.A. Boyd and Thomas Midgley, Jr., developed chemical means in the composition of fuel, yielding antiknock agents, notably tetraethyl lead, and fuels of high octane number, exemplified by triptane. This concept exerted a major impact upon the evolution of both the automobile and oil industries, and became adopted as a standard, still adhered to today, although use of additives has been replaced by the hydrogenation of fuel.

Semenov, the Nobel Prize Laureate for his contributions to the theory of chain reaction theory and Director of the Institute of Chemical Physics in Moscow, in collaboration with A.S. Sokolik, Ya.B. Zeldovich, L.A. Gussak, A.A. Borisov, V.P. Karpov, Yu. V. Tikhonov, and many others, set out over forty years ago to develop chemical-kinetic means for direct control of the combustion process, leading to the development of the LAG (Lavinnia Activatsia Gorennia or Avalanche Activated Combustion) Process (22). It is the principle established on this basis that warrants recognition as potential for a significant advance in combustion and engine technology, the LAG engine developed by Gussak being just but one of a whole array of possible solutions [vid. Dale and Oppenheim (23, 24)].

THERMOCHEMICAL AND GASDYNAMIC FEATURES OF KNOCK

EXOTHERMIC CENTER - To assess the relative merit of cures, one has to appreciate the thermochemical and gasdynamic features of knock. In essence, the phenomenon is due to a non-uniformity in the thermochemical state of the charge, as it is compressed in the cylinder prior to combustion. This is so, irrespectively whether the element of charge giving rise to knock is ahead, within, or behind the zone of the propagating flame front. As a consequence, there arise what is usually referred to as "hot spots", occurring more-or-less sporadically in the charge, prior to the consumption of their immediate environment by the combustion process.

Let us consider what exactly takes place under such circumstances. One should note first that a much more appropriate name for a "hot spot" is exothermic center. Its essential properties are displayed in Fig. 1. As demonstrated on the time-space diagram at the right side, the center consists of a kernel, the site of the exothermic chemical reaction, and of surroundings subjected to the pressure wave generated by the expansion of the kernel as well as the heat it transfers out. By virtue of the relatively small size of the kernel, its initial radius being in the mm range (25), temperature and concentration gradients within its boundaries can be neglected and the process inside considered as spatially homogeneous. Time-wise evolution of the exothermic energy in the kernel and the concomitant power pulse are depicted on the left side.

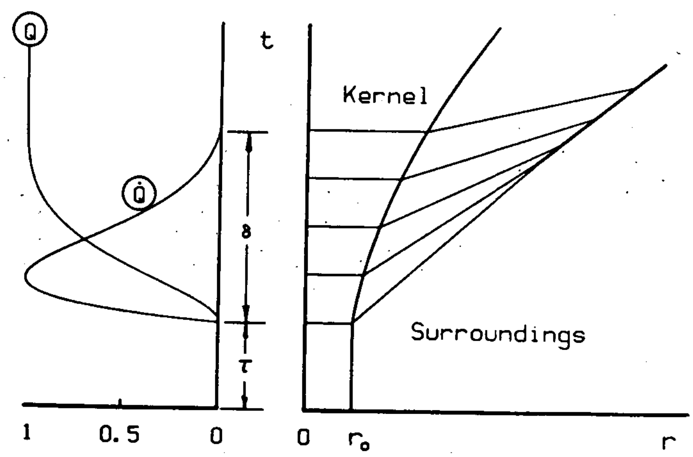

Fig. 1 - Essential properties of an exothermic center

The thermodynamic process occurring in the kernel over a differential step in time is presented on the so-called Le Chatelier diagram in Fig. 2. Displayed there on the left is the internal energy-temperature plane, and, on the right, the equivalent enthalpy-temperature diagram, each illustrating the same energy equation which can be expressed either as

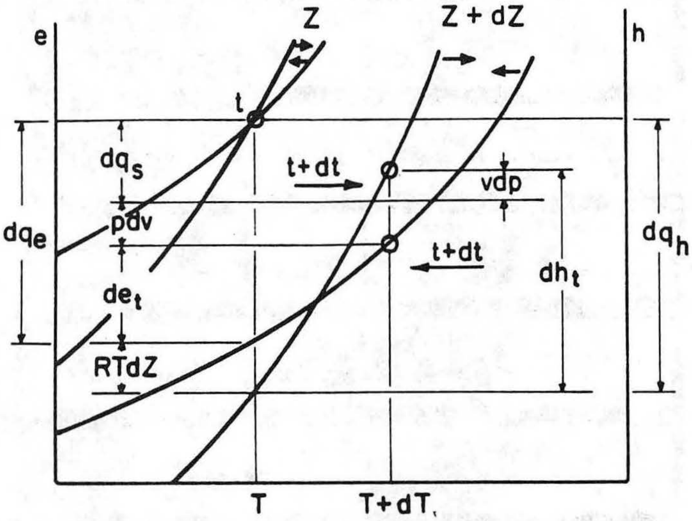

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Fig. 2 - The Le Chatelier diagram of the thermodynamic process occurring in the kernel of an exothermic center

$$dq_e = de + p\,dv + dq_s \tag{1}$$

or as

$$dq_h = dh - v\,dp + dq_s \tag{2}$$

where the symbols have the conventional meaning (e-internal energy, h-enthalpy, p-pressure, v-specific volume, t-time) whereas dq_e is the exothermic energy evolved in the interval t and $(t + dt)$, dq_h is the equivalent exothermic enthalpy, while dq_s is the concomitant heat transfer from the kernel to the surroundings. As marked on the diagram, the curves delineate lines of constant composition Z at t and $(Z+dZ)$ at $(t+dt)$. Specifically

$$Z \equiv \{(X_i) : i = 1, I\}$$

where X_i denotes the chemical symbol of given species, i=1,2,3...I, constituting the reacting mixture in the kernel, while the thick bracket indicates that its composition is expressed in the number of moles per unit mass. One should note that the specification of Z involves not only its value but also the identity of all its chemical constituents.

It can be shown [vid. Oppenheim (26)] that, as a consequence, the thermal source of the kernel can be expressed as

$$\frac{dT}{dt} = \mathring{Q} + \mathring{P} + \mathring{L} \tag{3}$$

where T expresses the temperature,

$$\mathring{Q} \equiv \frac{1}{\hat{c}_p} \sum_{i=1}^{I} [-\Delta h_i(T) \frac{d(X_i)}{dt}]$$

is the exothermicity rate,

$$\mathring{P} \equiv \frac{v}{\hat{c}_p} \frac{dp}{dt}$$

is the compression rate, and

$$\mathring{L} \equiv \frac{1}{\hat{c}_p} \frac{dq_s}{dt}$$

is the heat loss rate, each being essentially positive in the course of the expansion process - the essential part of the exothermic reaction. In the above

$$\hat{c}_p \equiv \sum_{i=1}^{I} [\tilde{c}_{pi}(T)(X_i)]$$

where h_i and c_{pi} are, respectively, the absolute enthalpy and specific heat at constant pressure of species X_i, while the tilde signifies that these quantities are expressed per unit mole.

Equation (3) reveals that the rate at which the temperature increases in the kernel is due not only to the exothermicity rate of the reaction, but also to the compression rate which, in turn, is governed by the volumetric rate of expansion of the kernel boundary. This brings forth the essence of the bootstrap runaway process of spontaneous ignition! As a consequence of the non-uniformity in the temperature of the charge, kernels of exothermic centers are formed in places where the temperature is at a local maximum, and, as they expand due to the consequent onset of an exothermic process within them forming a compression wave in the surroundings, the temperature is increased still further by virtue of the additional effect due to the rate of compression, enhancing thus, in turn, the rate of chemical reaction. This constitutes a runaway process of explosion (or, perhaps better here, micro-explosion) - an interesting case where loss of energy contributes towards the escalation of the process.

This is not all. In contrast to the conventional thermodynamic processes, the change of state taking place in the expanding kernel of an exothermic center has the unique feature of progressing along a line of simultaneously increasing pressure and specific volume. The surroundings, on the other hand, behave in the conventional manner, their process being not much unlike one at constant entropy. Consequences of this feature are demonstrated on the pressure-specific volume and temperature-entropy diagrams in Fig. 3.

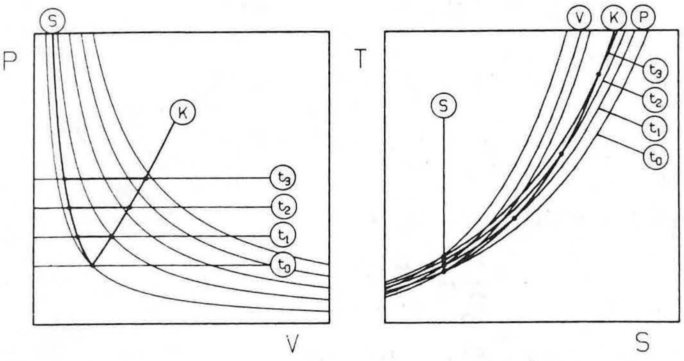

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Fig. 3 -Pressure-specific volume and temperature - entropy diagrams depicting the processes on two sides of the interface of an expanding kernel of an exothermic center

Noting that lines of constant pressure are also lines of constant time, it becomes evident from them that along the interface between an expanding kernel and its surroundings

$$\left(\frac{dT}{dt}\right)_{kernel} > \left(\frac{dT}{dt}\right)_{surroundings}$$

amplifying the runaway nature of the process.

MILD AND STRONG IGNITION - The thermal source of ignition, as expressed in terms of Eq.(3), has evidently two limiting cases:

(1) mild ignition occurring when $\dot{p}$=0 while $\dot{\ell}$>0, and

(2) strong ignition arising when $\dot{\ell}$=0 while $\dot{p}$>0.

The most convenient way to study experimentally these modes of spontaneous ignition is by the use of reflected wave technique in a shock tube. An example of mild ignition is shown in Fig. 4, while that of strong ignition is presented in Fig. 5. Both were obtained by the use of laser-schlieren cinematographic technique with the same stoichiometric iso-octane/oxygen mixture diluted by argon at two different initial temperatures (27). As demonstrated by these records, at a lower temperature, Fig. 4, spontaneous ignition is manifested by the generation of discrete flame kernels, while at a higher temperature, Fig. 5, the exothermic process progresses homogeneously throughout the compressed mixture behind the reflected wave, forming a blast wave headed by a shock front which is quite distinct right from the outset.

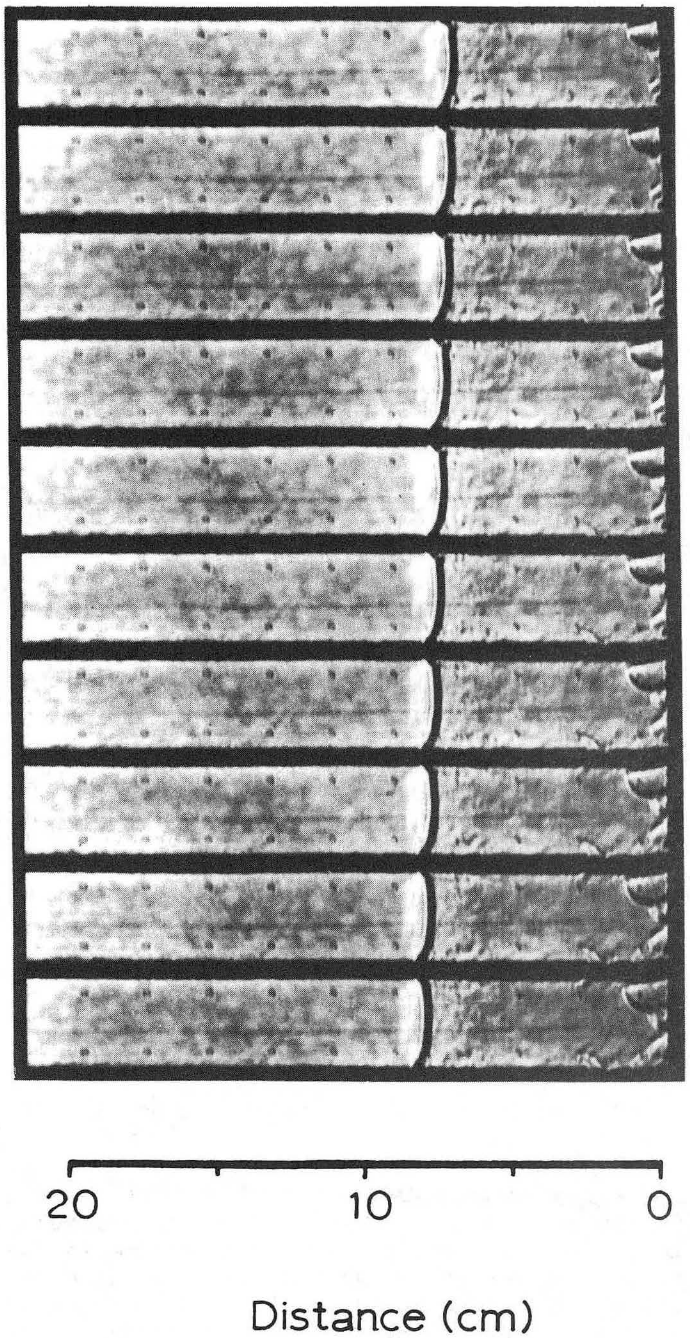

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Fig. 4 - Example of a mild ignition

End wall of tube at right edge of field of view
Sequence from top at time intervals of 2 μsec between frames

There is, of course, a line of demarkation between the regimes of the two modes of ignition. It is referred to as the strong ignition limit, and displayed for n-heptane in Fig. 6 and for iso-octane in Fig. 7, both taken from the paper of Vermeer et al.(27). As they appear there, strong ignition limits for these hydrocarbon systems are virtually independent of pressure, a feature indicative of the fact that, with reference to Fig. 1, the duration of the power pulse, δ , is, for these mixtures, proportional to the induction time, τ.

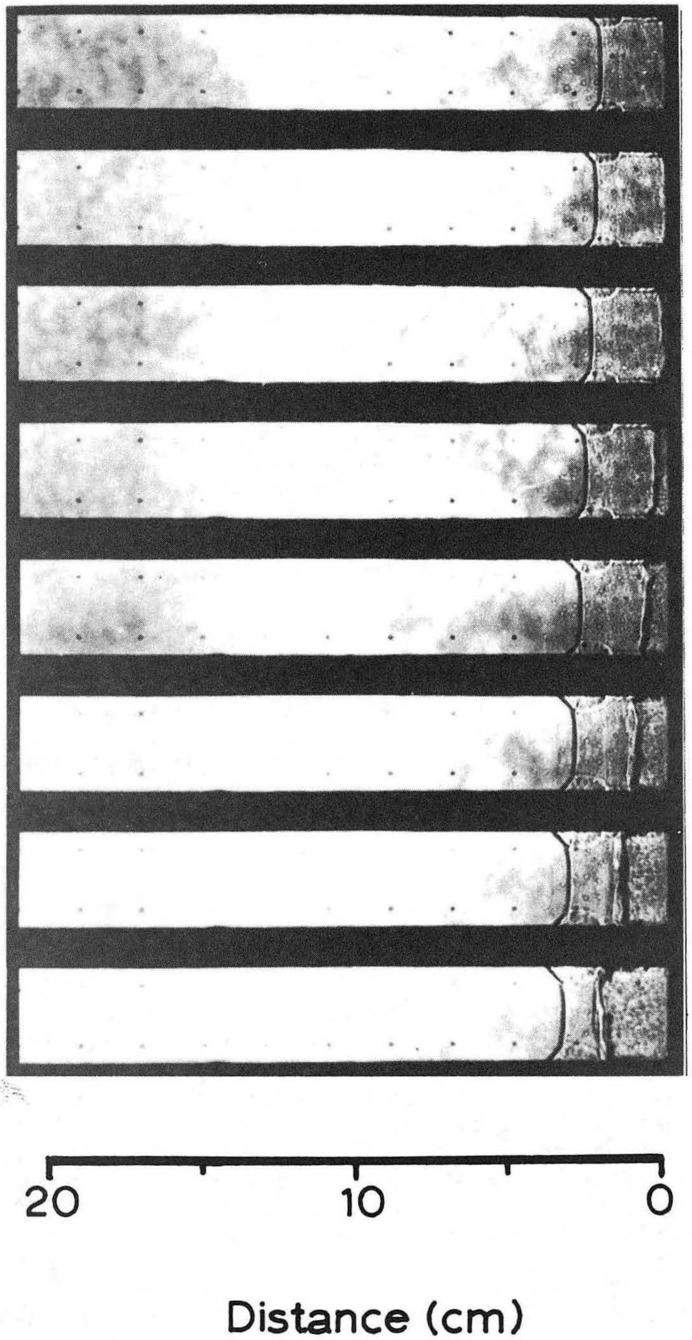

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Fig. 5 - Example of a strong ignition

End wall of tube at right edge of field of view
Sequence from top at time intervals of 2 μsec between frames

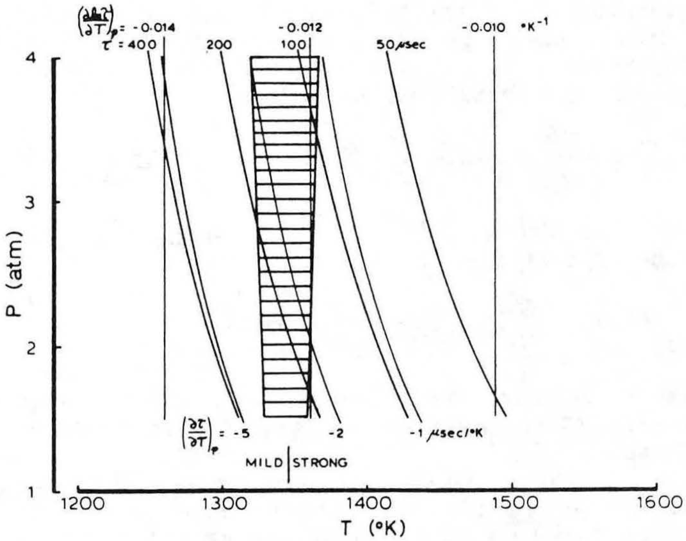

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Fig. 6 - Strong ignition limit for n-heptane

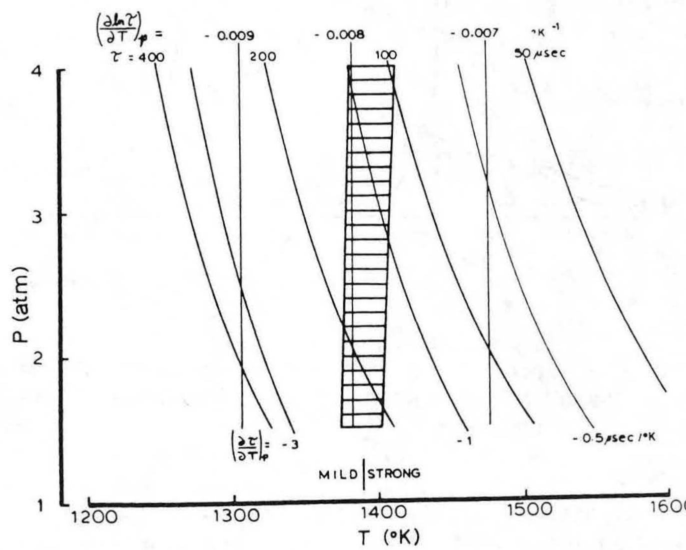

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Fig. 7 - Strong ignition limit for iso-octane

STOCHASTIC NATURE OF STRONG IGNITION - The phenomena described in the previous section with reference to Figs. 4-7 could not have been produced, of course, by a single exothermic center, but were generated rather by a relatively large set of such centers. The outcome, with respect to the question whether one gets mild or strong ignition, depends then on the coherence between the onset and duration of the exothermic power pulses of a set of more-or-less randomly distributed kernels.

Whereas a variety of more appropriate probability density functions for the exothermic centers could be taken into account, let us consider for illustration the simplest case of a Gaussian distribution of the temperature among a set of N kernels per unit mass, as done by Meyer and Oppenheim (28) who derived the following expression for the resulting power pulse

$$\dot{Q} \equiv \frac{dQ}{dt} = \frac{1}{2}\left[erf\left(\frac{\theta-\theta_m}{\sqrt{2\pi}}\frac{\delta}{\omega}\right) - erf\left(\frac{\theta-\theta_m-1}{\sqrt{2\pi}}\frac{\delta}{\omega}\right)\right] \quad (4)$$

Here $Q \equiv q(t)/q(\delta)$, $\theta \equiv t/\delta$ and $\theta_m = \tau_m/\delta$, subscript m denoting the mean, while

$$\omega \equiv (-\partial\tau/\partial T)_p\,\sigma$$

is the standard deviation in the induction time, whereas σ is the standard deviation in the temperature.

A plot of Eq.(4) for various values of ω, expressed in terms of their ratio to δ, is presented in Fig. 8. Displayed at its right is the dependence of the maxima of the power pulses on standard deviation in temperature for the particular case of $(\partial\tau/\partial T)_p = -2$ msec/K while $\tau = 2$ msec, typical conditions encountered in the vicinity of strong ignition limits. As evident from the latter, a deviation of only 4°C, at a level of 1000 K, is associated with a tenfold decrease in maximum exothermic power with respect to that obtainable in the case of uniform initial temperature distribution. Thus, relatively small deviations from uniform temperature have a significant effect upon the exothermic power pulse or, in other words, to get strong ignition from a given mass of a reacting mixture, one needs an amazingly constant temperature throughout the charge of combustible mixture.

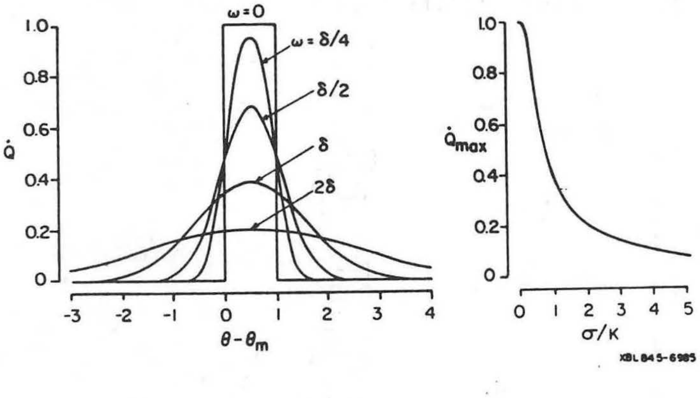

Fig. 8 - Dependence of the exothermic power pulse upon standard deviations in the induction time and in the temperature

It should be noted that, in the above, strong ignition has been identified with the phenomenon of knock. The two are indeed physically identical. The practical question one may have at this point is what specifically are the critical conditions for the onset of knock. As it should be obvious from the foregoing, the answer to this question is that, at their most rudimentary level, one should be able to express such conditions in terms of the maximum power of exothermic energy and its amount. On the plane of coordinates expressing these two quantities, critical conditions should appear as, roughly, a hyperbola. The larger the maximum power, the smaller should be the required amount in order to promote strong ignition or knock.

As evident from the above, these notions are as yet in their formative stage. It is the task of their specification that should provide the most significant objective for a most fruitful study of knock - an effort that should yield information one needs not only to develop proper means for the annihilation of this syndrome as a destructive phenomenon, but also for its exploitation as the actual source of power.

IMPLEMENTATION

The essential feature of proper means for the elimination of the syndrome of knock is quite straightforward: development of combustion systems operating in a knock-controlled mode, that is, systems where the occurrence of the destructive effects of knock are prevented by actually allowing the phenomenon to take place but only in the form of a great multitude of miniscule, properly distribued in time, micro-explosions.

The fundamental concept of such systems has been described in one of our previous papers (24) as that of a homogeneous combustion process. Its modus operandi is depicted in Fig. 9 taken from that paper. The basic principle involved here is simply that, instead of allowing the combustion front to sweep across the mass of the charge, the exothermic process is distributed in such a way that it proceeds, in effect, homogeneously throughout the charge.

The former, conventional case of what is best referred to as solitary flame is presented in Fig. 9a. The latter, in its purest form, is shown in Fig. 9b. The rest of the diagrams portray mixed cases. Figure 9c illustrates that of an end-gas knock, and Fig. 9d the opposite process of homogeneous ignition forming a solitary flame, as it occurs for example with the use of jets (27,28,29). Each is, in effect, a mixture of the elementary processes of Figs. 9a and 9b. Finally, Fig. 9e provides an example of a system consisting simply of a multitude of flames, each being, essentially, that of Fig. 9a, whereas Fig. 9f represents a system made up of a set of distributed exothermic centers, giving eventually rise to a multitude of flames, each being basically that of Fig. 9d ("multitude" is meant here to imply a number of an order of 10^n where n>>1). Both have the operating properties of the homogeneous combustion system of Fig. 9b, and describe thus practical ways in which such a system can be realized.

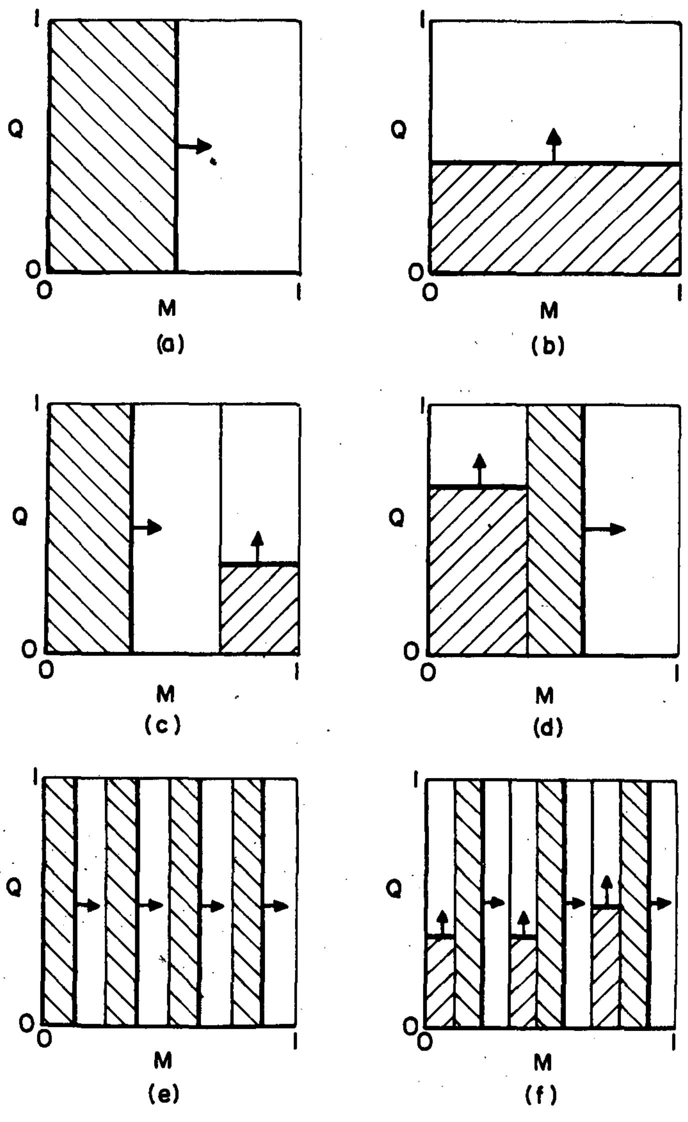

Fig. 9 - Modus operandi of systems operating on the principle of homogeneous combustion in contrast to that of a solitary flame

As implied above, in principle the syndrome of knock can be abetted by the development of systems operating on a homogeneous combustion process - the most appropriate means for the realization of controlled combustion, equivalent to controlled explosion, or controlled knock, all three terms being, in effect, synonymous. The elementary components of such systems may consist of such devices as:

1) combustion jets, exemplified by the LAG engine (22) and the flame jet ignitors (32,33),
2) plasma jets, exemplified by the studies of Weinberg et al. (34), Dale et al. (35) Oppenheim et al. (27,28,29), Asik et al. (36), and Dabora (37),
3) prompt exhaust gas recirculation exemplified by the systems of Onishi (38), and Nogushi et al. (39), as well as the experiments of Najt and Foster (40),
4) prompt residual gas utilization exemplified by the NAHBE engine of Pouring (41,42) and, in a potential form, by the Fireball engine of May (43,44).

Homogeneous combustion systems offer a number of significant advantages, namely:

1) complete elimination of knock by virtue of the essentially knock-controlled mode of operation, optimizing thereby engine tolerance to a wide variety of fuels,
2) maximization of efficiency by allowing the engine to operate at a relatively high compression ratio, combined with the beneficial effects of dilution on the cycle efficiency. The latter is demonstrated by Fig. 10 presenting the thermal efficiency of an Otto cycle for a hydrocarbon/air mixture, η, as a function of the dilution factor, ξ, a parameter of quite a general meaning, that is

$$\xi = \phi \equiv \frac{(A/F)_{\text{stoichiometric}}}{(A/F)}$$

or

$$\xi = \psi \equiv \frac{1}{1-(G/A)} = 1 - f$$

where A, F and G denote, respectively, the mass of air, fuel, and gas in the charge, while f is the conventional expression for the gas to charge ratio,
3) minimization of the generation of pollutants as a consequence of the distribution of the oxidation process into small parcels of charge to assure its completion within the required time, as allowed by engine speed,
4) performance at lower peak pressures and temperatures with concomitant benefits in structural and coolant requirements,
5) remarkably stable operation as a consequence of the stochastic effect of the multiplicity of ignition sources, resulting in complete elimination of cycle-to-cycle variations - a feature which renders the performance of the engine fully compatible with all the benefits, so readily available today, of electronic control systems.

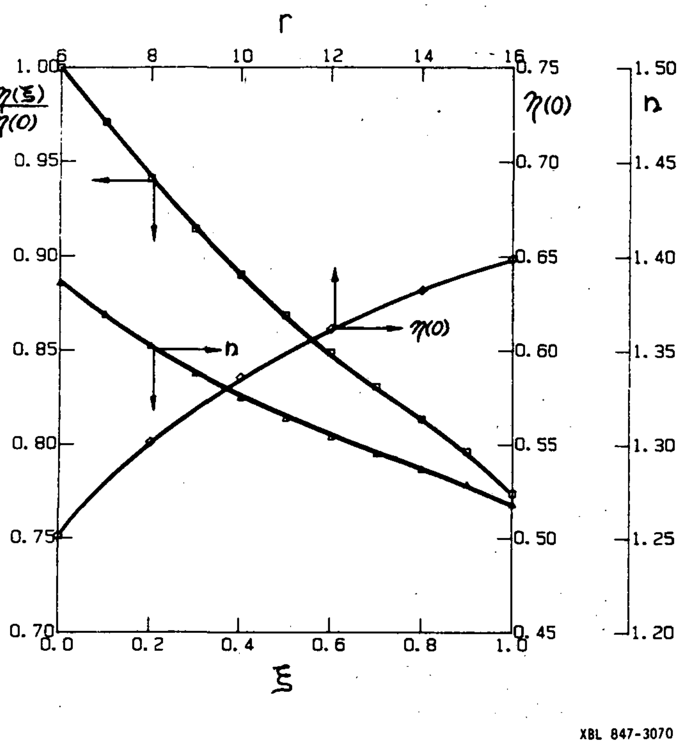

Fig. 10 - Thermal efficiency of an Otto cycle as a function of a generalized dilution factor

$\eta(\xi)/\eta(0)$ plotted on the diagram has been evaluated for a methane/air mixture at r=8 while $\xi=\emptyset$; the corresponding dependence of $\eta(0)$ on the compression ratio, r, is provided also, so that $\eta(\xi,r)$ could be estimated by multiplying the two; for other hydrocarbons use can be made of the effective polytropic exponent, $n(\xi)$, presented on the diagram, whence $\eta(\xi,r) \approx 1-r^{1-n}$

There are, of course, also some important disadvantages, namely:
1) relatively low specific torque and power density,
2) relatively low volumetric efficiency - a concomitant feature of the above, and
3) relative inflexibility of operation, making variable load performance difficult to control, as well as
4) relative novelty of the concept with all the imponderable problems its implementation may invoke.

One should realize that these disadvantages are essentially against the sense of direction pursued for over a hundred years by the automotive industry. Their gravity is, indeed, so significant that it may rule out any effort towards practical realization of the concept of homogeneous combustion systems.

VICTIMS

As pointed out in the introduction, the problem of knock imposes the major technical constraint upon the evolution of automotive technology. The victims of the lack of a satisfactory solution to this problem are then all the people who derive any benefit from the automobile, as well as those who are exposed to its effects. In a modern world, not much is left out.

Most prominent among such victims are then:
1) the modern society, so dependent upon the automobile and at the same time so abused by the burden of an unnecessarily too expensive fuel and the effects of pollution,
2) the automobile and oil industries, so affected by the knock syndrome that, instead of attempting to solve the problem, could do no better than to learn, at a considerable expenditure of time and money, how to live with it by establishing the octane rating of fuels and developing adequate means to comply with its standard, and
3) most of the research and development effort in this field that takes for granted the fact that the operation of an internal combustion engine must be based on the use of a solitary flame which, in order to accomplish its task of conducting the combustion process, has to sweep across the whole mass of the charge.

CONCLUSION

According to the arguments presented here, combustion technology may be advanced in our life-time by a quantum jump, comparable in significance to that exerted by the advent of transistor upon the electronic industry, or it may remain essentially unchanged. Admittedly, the probability of the former is much lower than of the latter, but this does not mean that it should be completely ruled out. In the event that a significant progress in combustion science is indeed made, it is most likely that it will first affect the automotive technology, because the automobile engine offers the greatest challenge for the most advanced application of combustion. The way in which the actual advance will be made should be in the form of a homogeneous combustion system, for, in contrast to flame-based systems we have today, it provides the most appropriate means for control of the process in the course of its progress - a feature that lends itself to all the benefits provided by modern electronic controls.

The homogeneous combustion system operates de facto on a knock-controlled mode, constituting a distributed set of micro-explosions or micro-knocks, so that the control is actually attained by following the adage of Julius Caesar: "Divide et Empera!"

In closing, I wish to confess that my motivation for this paper stems from the belief that the era of giants who almost singlehandedly could affect the progress of industry, as illustrated here earlier, is gone. The most a man can expect to accomplish is to be a catalizer or an inhibitor. Obviously I prefer to be the former. It is also my belief that today too much effort is spent in combustion research on some problems for the sole reason that they are considered to be unsolved. Thus, imparting a sense of direction to enhance the progress of technology should be beneficial to all parties concerned. It is towards this objective that our previous papers (vid. refs. 23 and 24), as well as this one, were directed. The concepts put forth here are as yet premature to launch a program of engine development. However, they are certainly sufficiently advanced to be taken seriously under consideration. In spite of the tongue-in-cheek attitude I adopted to attract attention, most of the statements made in the paper are scientific in nature and thus, as Karl Popper said, subject to refutation. Consequently, if the only result the paper attains will be a debate, I would consider its objectives well fulfilled. After all, this would be more than can be said about our previous papers.

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