THE ONSET OF KNOCK IN GAS FUELED SPARK IGNITION ENGINES PREDICTION AND EXPERIMENT

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Abstract

An approach for predicting the onset of knock and estimating its intensity in spark ignition engines is described. It is based on evaluating a dimensionless energy functional group, Kn, formulated to provide a numerical criterion to test continually, while using predictive models of the performance of spark ignition engines, for the onset of knock and its relative intensity at any instant during the combustion process. The basis for the derivation of this knock criterion and its significance are described. Examples involving gaseous fuels and their mixtures under different operating conditions show how the criterion can be employed for the prediction of the onset of knock and the associated knock-limited performance. It is shown that this approach can be made an integral part of modeling spark ignition engine operation to be used for optimizing engine performance while ensuring throughout the avoidance of the onset of knock.

Among other things variations relative energy release and end gas mass fraction during flame propagation for non-knocking and border line knocking conditions, variations in the calculated knock criterion value with time for knock free, light and heavy knocking conditions, with compression ratio for hydrogen and methane as a fuel CFR engine, calculated optimum spark timing maximum power variation the probability of the incidence of knock versus spark timing, the suppression of the onset of knock through lean operation or cooled EGR are illustrated in the paper.

Keywords: *combustion engine, gas engine modelling, engine performance knock criterion*

Nomenclature

CR	- Compression Ratio
Kn	- Knock Criterion
Φ	- Equivalence Ratio
Φkn	- Knock Limited Equivalence Ratio
Φop	- Operation Limited Equivalence Ratio
$\Delta\theta c$	- Combustion Duration, °CA
$\Delta\theta$c, ref	- Reference Combustion Duration, °CA
$\Delta\theta$c,f.c.	- Combustion Duration for Fast Flames, °CA
Δho	- Effective Heating Value of the Fresh Charge, kJ/kg
Hsp	- Enthalpy of the Mixture at Spark Timing, kJ/kg
ht	- Enthalpy of the Mixture at any Instant "t", kJ/kg
*m*o	- Mass of the Fresh Charge, kg
mu	- Mass of the End Gas at any Instant "t", kg
xi	- Operational Variable, *i*

1. Introduction

The uncontrolled combustion phenomenon commonly encountered in spark ignition engines known as "knock", is associated with exceedingly high rates of energy release, heat transfer and

pressure rise that must be avoided to ensure acceptable and safe engine operation. Knock imposes very serious limits to the increase in power output, efficiency, type of fuel that can be used and any further reductions in emissions in spark ignition engines. If an engine is allowed to continue running in a knocking mode for long, serious mechanical and thermal damage may ensue. Every effort is usually expended in the design, operation and control of S.I. engines to reduce the likelihood of the onset of knock to an absolute minimum. Often, this means that for any engine and fuel, the design and operating variables are selected conservatively to ensure knock free operation while sacrificing the potential optimum performance of the engine and fuel combination. If effective means can be found to predict the likelihood of the onset of knock for any set of operating conditions of the engine with a fuel, then protective measures can be devised more precisely while ensuring throughout optimum knock-free performance.

The phenomenon of knock in spark ignition engines results from the uncontrolled rapid energy release well ahead of the turbulent propagating flame front, due to autoignition of part of the unburned fuel-air mixture. This autoignition is the outcome of a complex interaction that takes place between the flame propagation processes and the preignition oxidation reactions of the end gas region of the mixture that is yet to be consumed by the flame.

The prediction of the onset of knock thus far has not been easy and effectively no relatively simple yet reliable approaches have been developed for quick and systematic applications including optimization approaches. This is because the prediction of the onset of knock in spark ignition engines requires a detailed knowledge of the transient state of the unburned mixture and its accelerating reaction activity. The extent of the preignition reaction activity needs to be followed closely and its consequences for the combustion process and the corresponding engine behaviour established. A very wide range of attempts have been made over the years to formulate such models (e. g. 1 to 11). These have tended generally to be limited in their scope, either fuel and engine specific or lacked accounting in sufficient detail for the reactivity of the temporally changing end gas region. However, the availability of increasingly fast and large capacity computers together with the enormous progress made in combustion science in general and chemical kinetics in particular, make it increasingly possible to devise successfully predictive models that can validate well against corresponding experimental results. The present contribution describes a unified formulation. The model is relatively simple and based on the value and rate of variation in the calculated value of a dimensionless energy function that can be used to monitor at any instant the closeness of the instantaneous mass of the end gas to the onset of end gas autoignition and knock.

2. Background

In an engine, following external spark ignition, the propagation of the turbulent flame front throughout the whole mixture needs to be completed before any part of the unburned cylinder charge undergoes autoignition. Should the propagating flame not manage to consume the entire mixture in time before autoignition takes place somewhere within the mixture yet to be burned by the flame, commonly known as the “end gas” region, then a sudden rapid and intense energy release takes place that can be detected as spark ignition engine knock. The intensity of this knocking condition can be readily detected through measures such as monitoring the rapid change in the rate of cylinder pressure rise, the distinctive noise emitted, a rapid drop in power output and efficiency, excessive heat loss to the walls and changes in the exhaust emissions and temperature. The intensity of the resulting knock can be related to the associated intensity of the resulting rate of pressure rise. This in turn will be a function of the net energy released by autoignition which mainly controls the intensity of the temporal changes in cylinder pressure. These are dependent mainly on the mass of the end gas undergoing autoignition and the cylinder volume at the time.

The onset of autoignition and the associated extremely rapid energy release rates within a

homogeneous fuel air mixture are normally the outcome of rapid acceleration of the preignition chemical reaction activity due to the gradual increase in temperature and pressure and the build up of concentrations of active species that are mainly of the radicals' type. Various indicators may be employed to define the end of the ignition delay. These may include the observed rapid changes in temperature, pressure or the concentration of some active species within the mixture that help in the rapid propagation of the overall reaction, such as the radical ”OH”. Often, it is easier to associate the termination of the ignition delay with the consumption of a certain fraction of the fuel or oxidant or the release of a certain fraction of the exothermic energy of the oxidation process. These different approaches can be shown to yield when used essentially similar values for the delay, [12].

Autoignition of the mixture within the end gas region of the engine cylinder is the outcome of the complex interaction of the chemical processes that are controlled by the numerous operating and design variables. Accordingly, any relatively simple approach to the prediction of the onset of knock and its resulting intensity must necessarily incorporate numerous simplifying assumptions. However, in view of the dominant role of the chemical kinetics of the preignition reactions processes their full representation must be employed. The present approach incorporates such a detailed representation.

3. The Model

3. 1. Modelling S.I. Engine Performance

A two-zone and quasi-dimensional model that predicts the performance of S.I. gas engines and can include the testing for the onset of knock should it occur has been described, [Bade Shrestha and Karim, 1999(a)]. In this approach the homogeneous charge of the cylinder is assumed at any instant during turbulent flame propagation combustion to be divided into two zones of burned products and unburned reactants that include the end gas region. The intake stroke is simulated while accounting for the presence of residual gases. The simulation for the other strokes is based on the state of the mixture at the end of the intake stroke. Changes in the unburned reactants are evaluated up to the time of spark ignition while accounting for the heat transfer between the fuel mixture and surrounding walls. An appropriate combustion energy release pattern over the entire combustion period is employed to simulate the combustion and the corresponding energy release processes after ignition. Following examination of a large number of experimental data for a variety of operating conditions, it was shown that a triangular function would be quite adequate for the present modelling approach [Bade Shrestha and Karim 2001 (a)]. The combustion duration and lag time model was validated against corresponding experimental data. The composition of the burned products following flame propagation is calculated while accounting for thermodynamic dissociation. In the absence of specific information about heat transfer from the two combustion zones to the outside walls with hydrogen combustion, a formulation [Woschni, 1967] that was based on experimental observations made in hydrocarbon fuelled engines was incorporated in the modelling. In order to monitor at any instant during flame propagation the likelihood of the onset of knock due to autoignition of the unburned end gas, the reactivity of the temporally changing end gas region is evaluated employing a sufficiently detailed description of the chemical reaction kinetics of the unburnt mixture.

3. 2. Accounting for the Incidence of Knock

At any instant during flame propagation, the energy released by the preignition reaction activity of the current size of the unburned charge, can be calculated using detailed chemical kinetics, needs to be normalized to take into effect the influence of the prevailing operating and design conditions. This fractional exothermic energy release by preignition reactions of the end gas

per unit of the instantaneous cylinder volume may be normalized relative to the energy that would be released by normal flame propagation in the absence of knock per unit of initial cylinder volume at the beginning of compression. The resulting dimensionless energy function $K_{n,}$ being described as the *criterion for the onset of knock* is defined by equation (1).

$$K_n = \frac{\dfrac{\text{Total Energy Released Due to End Gas Reactions up to Time 't'}}{\text{Cylinder Volume}\big|_t}}{\dfrac{\text{Total Energy of the Whole Charge to be Released by Flame Propagation}}{\text{Cylinder Volume}\big|_{t_o}}} \quad . \tag{1}$$

The numerical value of this dimensionless criterion, *Kn*, represents the relative intensity of the energy released by the preignition reactions leading to autoignition of the fractional mass of the diminishing end gas at the time, t, when normalized relative to the total energy released by combustion through flame propagation. Since it would be reasonable to assume that the manifestation of knock will be affected by the size of the cylinder at the instant of autoignition relative to the cylinder size represented by its volume at the beginning of compression, the numerical value of this dimensionless criterion *Kn* can indicate a quantitative measure of the tendency of the charge to experience knock at that instant of time. Moreover, its value beyond a threshold for ignition will be indicative of the relative energy release by the autoigniting mass and hence of the approximate intensity of knock when it does take place. The effects of flame propagation, heat transfer and changes in volume due to piston motion are accounted for within the calculated chemical energy release that is cumulatively a function of the temporal changes in temperature, pressure and composition. The preignition reaction activity and its energetic consequences can thus be continuously evaluated and followed with time using sufficiently detailed chemical kinetics. A critical value of this dimensionless function, *Kn*, will be associated with the threshold of the incidence of knock. Thus, it can be seen that the changing numerical value of the dimensionless criterion, *Kn*, at any instant during the combustion process in an engine is a product of the fractional combustion energy released by preignition reaction activity that may lead to autoignition times the fractional mass of the end gas and amplified by the engine compression ratio. The value of *Kn* will be very small when a negligible amount of preignition reaction energy is released, the compression ratio not too high and/or when the mass of the autoigniting end gas is fractionally too small.

The criterion, *Kn,* as defined by equation (1), also can be shown to correspond at any instant of time, t, to the calculated fractional pressure rise exclusively due to the energy release by the preignition reactions of the instantaneous mass of the end gas normalized relative to the combustion mean effective pressure. This latter pressure is defined as the total energy of combustion per unit of engine cylinder initial volume.

The form of the criterion shown in equation (1) may be simplified so as to incorporate more recognizable variables that reduce *Kn* to the following form:

$$K_n = \frac{h_{sp} - h_t}{\Delta h_o} \times \frac{m_{u,t}}{m_o} \times (CR - 1)\,, \tag{2}$$

which is the product of the calculated fractional energy released from the preignition chemical reactions of the current size of the end gas at any time, t, calculated using detailed chemical kinetics and its fractional mass amplified by the compression ratio. The critical value of this simplified form of the criterion at the onset of borderline knock was found experimentally in the CFR variable compression ratio engine for a wide range of operating conditions to be around 1.0 to 1.5. This would imply that for a typical compression ratio of 10:1, the product of the fractional mass of the end gas and the fractional energy release by the reactions to be around 0.10 to 0.15, depending on the set tolerable level of the intensity of knock. Such a relatively simple knock

modelling approach that incorporates detailed chemical kinetic calculations

$$K_n = \frac{h_{sp} - h_t}{\Delta h_o} \times \frac{m_u}{m_o} \times (CR - 1) \times \frac{\Delta h_o}{(\Delta h_o)_{stoich}} \times \frac{\Delta \theta_{c,ref}}{\Delta \theta_{c,f.c.}}, \quad (3)$$

to evaluate "h_t", was shown to be capable of predicting successfully the onset of knock in S.I. engines fuelled with a range of gaseous fuels with some liquid fuels, [13]. However, for engine operation with pure hydrogen, much of the operation is carried out with lean mixtures and well away from the normal trend of stoichiometric operation with other common fuels. Moreover the flame propagation rates with hydrogen operation are much higher than those encountered with other fuels. Knock can be encountered over a much wider range of equivalence ratio values and with very widely varying flame propagation rates than with the other more common fuels. To improve the prediction of knock with hydrogen as a fuel, account for these differences was made in a refined extended definition of K_n. In addition to the above, the energy release can be normalized also relative to that of the stoichiometric mixture while the combustion duration, which is the inverse of the mean flame propagation rate, is normalized relative to a typical constant value, $\Delta\theta_{c,ref}$, such as that commonly observed for completing flame propagation within the common fuel methane (e.g. 50 °CA), for K_n to become of the form of equation (3) [14]. This value of K_n is essentially the same as that calculated according to equation (2) for common gaseous fuels but for pure hydrogen engine applications equation (3) tends to provide predicted results that are in better agreement with experiment [14].

3. 3. Turbo-charged Operation with EGR

The knock prediction model was extended further to account additionally the effects of turbo-charging and cooled EGR on the total energy to be released through auto-ignition and the resulting knock intensity, (Li and Karim, 2006). The effects of the performance of after compression and EGR-coolers on the temperature of the intake mixtures and accordingly the pre-ignition reaction of the unburned mixture were also accounted for. The modification to the model includes the incorporation of experimentally based correlations of combustion duration values with changes of EGR ratio.

For turbocharged spark ignition engine with cooled EGR, the energy density of the intake mixture would increase approximately proportionally with the boost pressure ratio and decreases with the application of EGR due mainly to the displacement of some of the air-fuel mixture by the recirculated exhaust gases. Accordingly, the effects of turbo-charging and EGR can be incorporated to modify the knock criterion of equation (2), to the following form:

$$K_n = \frac{h_{sp} - h_t}{\Delta h_o} \times \frac{m_u}{m_o} \times (CR - 1) \times PR \times (1 - R_{\mathrm{EGR}}), \quad (4)$$

where: *PR is t*he absolute boost pressure ratio and R_{EGR} : is the EGR Ratio, which is defined as the molar fraction of the recirculated exhaust gases in the intake mixture.

The application of this approach to predict the onset of knock is sufficiently general in principle to be applicable to both liquid and gaseous fuels. However, in view of current limitations to the reliable prediction of the chemical kinetics of the autoignition reactions of higher hydrocarbon liquid fuel mixtures in air, the present contribution has targeted gaseous fuel applications. Some limited applications to liquid fuels showed satisfactory agreement with experiment. Moreover, this approach is applicable to engines of different size, design and speed ranges. Much of the illustrative results to be shown in this contribution relate to the variable compression ratio CFR engine. Some limited demonstrations relating applications to other engines and speeds were generally equally satisfactory.

4. Some Results

The approach described for monitoring the calculated value of K_n during the course of the modelling of the combustion process to test for the onset of knock was incorporated into a relatively simple two-zone predictive model [15], that we developed for the combustion process and performance of a spark ignition engine. In this model the homogeneous charge is assumed to be divided during flame propagation in two zones: burned products and unburned reactants. The composition of the mixture of the unburned reactants that comprises the end gas region is usually known at all times up to the time of spark ignition since the fuel-air flow rates were closely metered and the presence of residual gas and heat transfer effects accounted for. An appropriate flame propagation combustion energy release pattern is employed based on formulations obtained following examination of a large number of experimental data for a wide variety of operating conditions. The energy release due to turbulent flame propagation would take place over a certain combustion duration that would start just beyond the spark ignition timing after a short ignition lag period when a significant amount of energy begins to be released and would end with the end of flame propagation. A formulation for the variation of the combustion duration with key operating influencing variables, based on mass of experimental data obtained and described in some detail elsewhere [16] for a number of fuels was developed. Such an approach was shown to yield temporal cylinder pressure development and key engine performance variables that were in good agreement with experiment. It provides also the temporal variations in the size and mean temperature of the unburned zone which permits calculating continuously with time using chemical kinetic modelling the preignition reaction activity within the end gas. This would then allow the calculation of the instantaneous value of K_n throughout the progress of the combustion process to ensure that its value would not exceed the critical threshold value.

The application of such a modelling approach could yield continuously at any instant the properties of the unburned end gas region. The values of the prevailing temperature, pressure and size of the reacting end gas are thus determined with their variations with time. The corresponding reactivity, species concentrations and the thermal consequences of any preignition reactions are evaluated using detailed kinetic schemes appropriate for the fuel-air end gas mixture while using the current values of its properties such as temperature and pressure. Knowledge of these key parameters and their temporal variation permits the calculation of the value of K_n function and its potential growth with time, as the size of the unburned zone continues to shrink due to the continued propagation of the turbulent flame throughout the charge. A suitable detailed chemical kinetic scheme of 155 reaction steps was employed for fuel mixtures containing the gaseous fuels, propane, ethane, methane and hydrogen in air for conditions relevant to those normally employed within engines, [13, and 15].

Figure (1) shows an example of the temporal variation of the calculated value of K_n as the flame propagation proceeds consuming the cylinder charge. Two cases relating to a non-knocking and a border-line knock conditions are shown, [13]. The corresponding calculated variations in the fractional mass of the end gas and the preignition reaction energy release are shown. Figure (2) also shows a variation in the calculated value of K_n with changes in spark timing advance that bring about knock and increased its intensity with increasing the advance value. The onset of knock observed experimentally and its borderline intensity, appeared to correspond to a K_n value of around 1.5. Different operating conditions that were observed experimentally to produce borderline knocking were associated approximately with the same critical calculated value of K_n ,[13].

Figure (3) shows a comparison between the calculated lean and rich knock limited equivalence ratios for a range of compression ratios with the corresponding experimental values established for hydrogen operation in a CFR engine when using the form of the criterion of equation (4). Good agreement between the two sets of values can be seen throughout [14]. Such an approach when

integrated within a modelling procedure for predicting the performance of spark ignition engines can be employed to yield optimized knock free data for any specific engine-fuel combination while using a variety of optimization approaches including approaches based on genetic algorithm. Figure (4) shows the maximum variation in power output and the corresponding efficiency with variation in compression ratio when the equivalence ratio and spark timing are varied to obtain maximum power while just avoiding the incidence of knock (*Kn<1.5).* The corresponding efficiency variation is also shown to be of lower values than when conditions are chosen to achieve maximum efficiency, sacrificing somewhat the corresponding power output to maintain knock free operation [16].

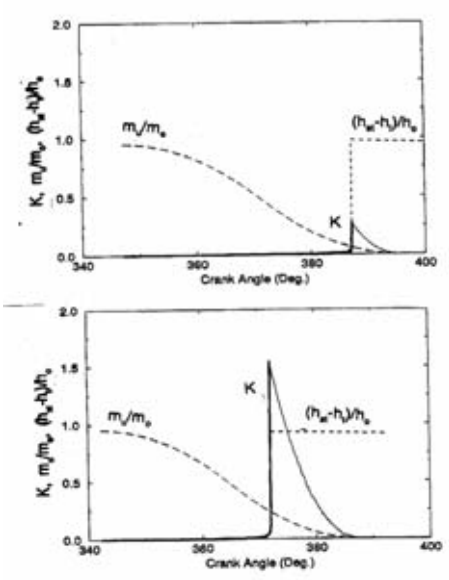

Fig. 1. Variations in the calculated value of K_n, relative energy release and end gas mass fraction during flame propagation for non-knocking and border line knocking conditions

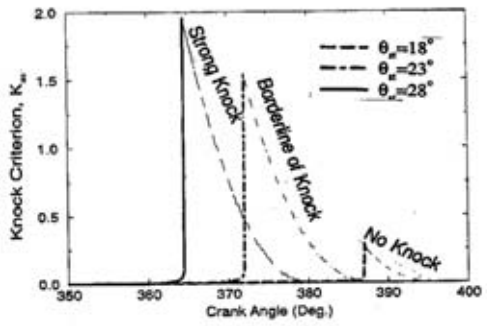

Fig. 2. Variations in the calculated value of Kn with time for knock free, light and heavy knocking conditions [17]

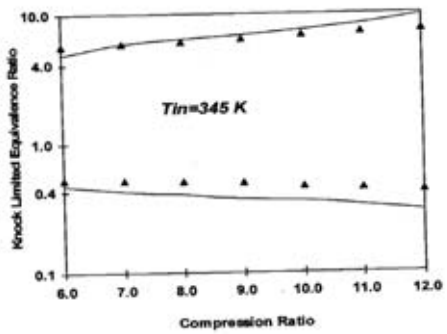

Fig. 3. Variation in the calculated knock-limited equivalence ratio with compression ratio for hydrogen CFR engine operation at an intake temperature of 345K; the corresponding experimental values are also shown, [14]

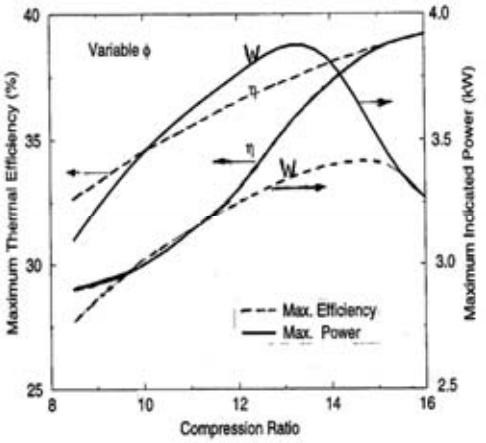

Fig. 4. Variation of maximum power and maximum efficiency with compression ratio for knock free operation with methane as a fuel in a CFR engine the corresponding efficiency and power, respectively are also shown, [17]

Another example of the application of the modelling approach is shown in Fig. (5) where the spark timing variation with compression ratio is shown for methane operation at an equivalence ratio of 0.90 and three different initial temperature conditions [17]. It can be seen that with increasing the compression ratio, the spark timing can be adjusted to maintain knock free operation even for very high compression ratios. The thick lines shows knock limited operation.

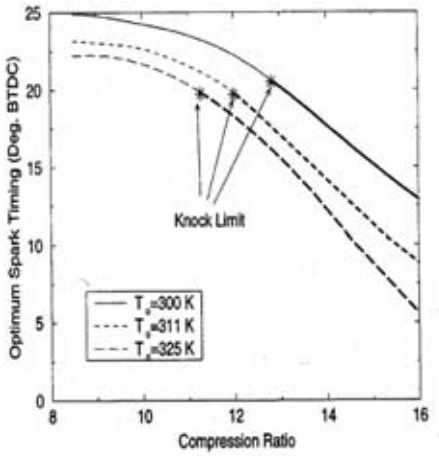

Fig. 5. Calculated optimum spark timing maximum power variation with compression ratio for three different initial temperatures at an equivalence ratio of 0.90 when operating on methane, thick lines indicate knock limited operation, [17]

Cyclic variation commonly encountered in engines is a complex function of the extent of any variation in the values of the many different operating and design variables that affect the course of the combustion process. Generally, this variation may be considered approximately random in nature. Traditionally, the observed variation in cylinder pressure temporal development or the value of the indicated mean effective pressure is used to indicate the extent of this cyclic variation. Similarly, the incidence of light knock does not take place initially in every cycle and is subject to cyclic variation. The probability of the incidence of knock at a given set of operating conditions, evaluated as the number of cycles knocking in a specified number of consecutive cycles, can be evaluated using the calculated probability in the variation of the value of the criterion, K_n. This latter variation is obtained through the application of equations (2) and (3) while incorporating the extent of variations in the key influencing variables [18]. Figure (6) shows an example of the calculated probability of the incidence of knock in one hundred consecutive cycles versus changes

in spark timing for a methane fuelled engine at a compression ratio of 14:1 and equivalence ratio 0.90, [18]. The steep dependence of the probability of the incidence of knock on the spark timing is evident. An advance of only 4 degrees in timing turned for this specific example a non-knocking condition into cyclically repeatable knock.

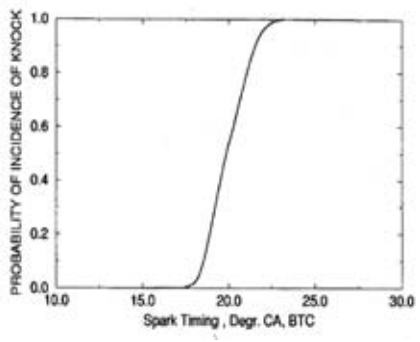

Fig. 6. The probability of the incidence of knock versus spark timing at compression ratio of 14:1, equivalence ratio of 0.90,To 294K,for methane operation, [18]

To get an engine out of a knocking state, a choice of changes to a number of operating conditions are possible. The following equation represents the reduction needed in the value of the criterion K_n under knocking condition to a lower borderline acceptable non-knocking value through calculated incremental changes to *Kn* due to the contribution of individual changes to the criterion when any operating variable *Xi* is only changed:

$$K_m - K_{c.} \leq \sum_{i=1}^{n} -\frac{\partial K_m}{\partial x_i} \Delta x \cdot \tag{5}$$

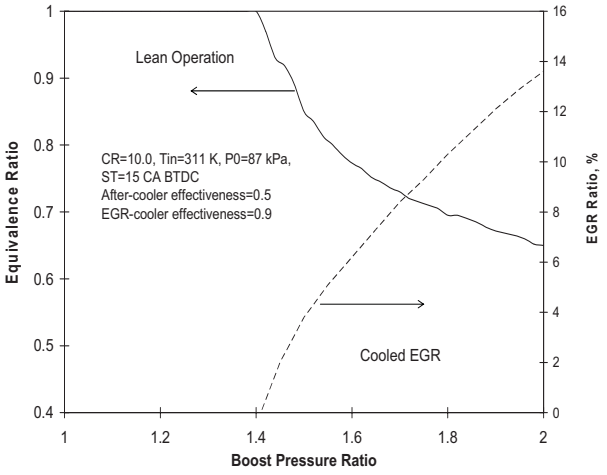

Fig. 7. The suppression of the onset of knock through lean operation or cooled EGR only. There is no EGR for lean operation. Equivalence ratio is kept at 1.0 when cooled EGR is applied. CR=10, ST=15 CABTDC, To=311 K, Po=87 kPa

Obviously, there is a large number of possible scenarios of changes to operating conditions that can be implemented to get out of a knocking condition. The selection of the optimum changes can be made analytically without necessarily excessive degradation to power or efficiency. This is made either through systematic evaluation of the consequence of a group of incremental changes to be made to key operating variables on the value of the calculated value of K_n or more elaborate mathematical optimizing procedures, such as the application of genetic algorithm applied. For example, at a border- line knocking condition, (K_n = 1.0) of a CFR engine operating on methane at

an equivalence ratio of 0.90 and a compression ratio of 12.0, a change in the value of *Kn* by a factor of one to render it knocking, (K_n = 2.0), can be obtained by individually changing the value of the equivalence ratio by merely 10.8%, the compression ratio by 0.43 or the intake temperature by 5.3 degrees, [13].

These are only a few typical examples involving gaseous fuel S. I. engine applications. They illustrate how through the use of this dimensionless function, K_n, modelling the performance of spark ignition engines can include the consideration of the possible incidence of knock. Its likely intensity can be indicated by the value of K_n. Procedures for getting out of a knocking condition also can be derived with the minimum of undermining power, efficiency or exhaust emissions.

Figure 7 shows an example of the application of equation (4) to a turbo-charged engine operating with cooled exhaust gas recirculation. It shows for any equivalence ratio the maximum knock limited boost pressure that can be employed with the extent of cooled EGR.

5. Conclusion

The occurrence of knock for any set of operating conditions can be established through calculation of the variation of the value of a dimensionless normalized energy group, K_n, while employing detailed chemical kinetic simulation for the end gas region of the cylinder charge. The maximum calculated value of K_n can provide an indication of whether knock is likely to be encountered or not, its timing and its possible intensity. Good agreement with experimental observations involving gaseous fuels was obtained. For the engine and fuels tested the threshold for the incidence of knock was associated with a maximum value of K_n of around 1.0 to 1.5.

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