A Criterion for Knock in Spark Ignition Engines

G.A.Karim and J.Gao*

Department of Mechanical Engineering
The University of Calgary
2500 University Drive N.W., Calgary, Alberta, T2N 1N4
Canada
* *NEWJEC Inc.*

ABSTRACT

The present contribution combines the consideration of the chemical reaction activity of the end gas and engine operating conditions to predict the onset of knock and associated performance in a spark ignition engine fuelled with methane. A two-zone predictive combustion model was developed based on an estimate of the effective duration of the combustion period and the mass burning rate for any set of operating conditions. The unburned end gas preignition chemical reaction activity is described by a detailed chemical reaction kinetic scheme for methane and air. The variation with time of the value of a formulated dimensionless knock parameter $\mathcal{K}$ is calculated. This parameter relates the total energy released within the end gas due to autoignition reaction activity per unit of the corresponding instantaneous volume relative to the total energy release per cylinder volume that would take place normally due to regular flame propagation. It is shown that whenever knocking is encountered, the value of $\mathcal{K}$ builds up to a sufficiently high value that exceeds a critical value. Under normal operating conditions, the value remains throughout the combustion period at comparatively low levels. The results produced were in good agreement with experiment in a laboratory engine.

NOMENCLATURE

A,B	constants, eq. 4
C	concentration
Cv	specific heat at constant volume
H,h	enthalpy
$\mathcal{K}$	dimensionless knock criterion
M	mass
P	pressure
Q	heat transferred
R	reaction rate
r	compression ratio
T	temperature
t	time
V	volume
x	function, eq. 5
x_i	concentrations of item i
y	function, eq. 6
α	number of species
θ	crank angle
ϕ	equivalence ratio
ρ	density

Subscripts

b	burnt, backward
c	combustion, end of combustion
f	fuel, forward
i	species, ignition
j	reaction step
L	lean limit
max	maximum
min	minimum
o	initial conditions
p	products
R	rich limit
r	reactants
s	spark timing
u	unburnt
t	time, t

INTRODUCTION

Interest in the efficient utilization of various gaseous fuel resources such as natural gas and other alternative fuels for the production of power has been increasing in recent years worldwide. This has been driven largely by the increased environmental constraints on engine exhaust emissions. The gas fuelled internal combustion engine with appropriate conversion and operational methods can have, in principle, performance characteristics that are as good as or may be made superior to those operating on conventional liquid fuels [1].

Ideally, for any engine installation when a certain gaseous fuel is used, the design and operating conditions need to be selected optimally so as to provide best performance over the entire load and speed ranges. No specific guidelines are usually available to designers, engine convertors and operators

to show how to deal optimally with any specific engine installation when operating on a specific gaseous fuel. This is especially the case in relation to the encountering of knock which can impose a severe barrier to engine output and the efficient utilization of some fuel resources in engines.

Guidelines are needed to show how the incidence of knock can be effectively dealt with and how to estimate for any engine and set of operating conditions, the limit for knock free output when employing any known combination of gaseous fuels. The present contribution describes a relatively simple approach for predicting the onset of knock in gas fuelled spark ignition engines. The results presented relate to conditions primarily while employing methane. Other fuels could have been similarly considered.

KNOCK LIMITED OPERATION

The knock phenomenon in spark ignition engines results from the autoignition of part of the charge ahead of the propagating turbulent flame [2]. Intense knocking is usually encountered when autoignition occurs regularly in every cycle and involves a significant portion of the charge [e.g.3,4]. There have been a number of attempts to predict the onset of knock, (e.g. 3). Specific guidelines convenient to use and especially in relation to gaseous fuels usage, are needed to help engine manufacturers, convertors, and operators avoid the incidence of knock in any specific engine and set of operating conditions. This is to be achieved preferably without reductions in power and efficiency nor increasing exhaust emissions.

The onset of knock in a spark ignition engine can be predicted in principle by assuming that knock is due to the autoignition of a region of the gaseous charge yet to be consumed by the flame while assuming its temperature variation with time is known. A representation of the autoignition reactions in a model based on a simple Arrhenius gross reaction is inadequate since the oxidation of the fuel-air charge for common fuels proceeds through chain reactions involving a sequential degradation of the reactants to eventual products via numerous intermediate species, both stable and unstable. For a relatively simple fuel such as methane, the nature and rates of these reactions have been established fairly reliably to yield good agreement with experimental observations, while using schemes involving a large number of simultaneous steps and species [5]. Kinetic schemes of other common fuels which are more complex than methane, are becoming increasingly available and their reliability is being steadily improved [6]. Obviously, such approaches add much to the computational complexity of the relatively simple conceptual model for knock prediction needed.

The end gas charge reactions will be critically dependent on the temperature and pressure variations with time. These variations are mainly controlled by the energy release rate due to turbulent flame development, a function of not only operating conditions but also engine design parameters, such as compression ratio and cylinder geometry. In the present contribution the effective temperature of the reactive end gas is established using for the cylinder charge a relatively simple two-zone model that assumes the transfer of mass from the unburnt to burnt zones at any instant through turbulent flame propagation takes place over an appropriate combustion period according to a deduced energy release rate function. These coupled parameters can be either known beforehand or established experimentally from a firing engine while employing a diagnostic two-zone model that analyzes the corresponding pressure-time development records [7].

PREDICTIVE MODEL FOR KNOCK

The decision as to whether knock is to take place and its intensity for any engine installation and operating condition with any fuel is a complex function of the cumulative effects of reactions proceeding within the end gas and how they are influenced by flame propagation and changes in the size of the end gas. Cyclic variability is also a common recurring factor in spark ignition engines and the temperature distribution within the end gas unlike that of pressure can be complex and non-uniform, especially once the engine begins to knock. Accordingly, only average values of operating parameters need be considered in any sample model for knock prediction and establishing the effectiveness of changes in operating and design conditions on the onset of knock and intensity.

The two-zone model developed avoids predicting the detailed features of turbulent flame propagation. Instead, through an appropriately assumed combustion period and associated mass burning and energy release rates, the changes in cylinder pressure and mean temperatures of the end gas and burned regions are established at any instant of time. These results are then employed to evaluate the extent of reaction activity ahead of the flame within the end gas and the associated energy release by such reactions. In time this would permit establishing whether autoignition will take place and the likely intensity of the resulting knocking.

In the model being considered, the cylinder charge is assumed during combustion to be divided into two zones: burnt products and unburnt reactants which comprise the end gas region, Figure (1). The contents of each of the two-control volumes are assumed for simplicity to be a mixture of ideal gases [8]. At any instant during the combustion process, mass is assumed to be exchanged only between the two control volumes. The composition of the mixture of the unburnt reactants is assumed known at all times up to spark ignition, since the fuel and air flow rates into the engine are closely metered and the presence of residuals accounted for. However, when considering the reactivity of the end gas detailed reaction rates and the associated reactive species are accounted for, together with the energetic consequences of such reactions. The composition of the burnt products as a result of flame propagation is calculated from a suitable temperature and pressure dependent dissociation scheme. Heat transfer from the two zones to the outside wall was accounted for using formulations recommended by Woschni [9] following analysis of a range of experimental data in engines.

The energy equation for the whole charge at any instant of time t, corresponding to a crank angle, θ, is:

$$dQ = d(M_u Cv_u T_u + M_b Cv_b T_b) + PdV \qquad (1)$$

where dQ is the net heat transfer that includes the energy release due to combustion treated for convenience as an extra heat addition as well as actual external heat transfer through the walls.

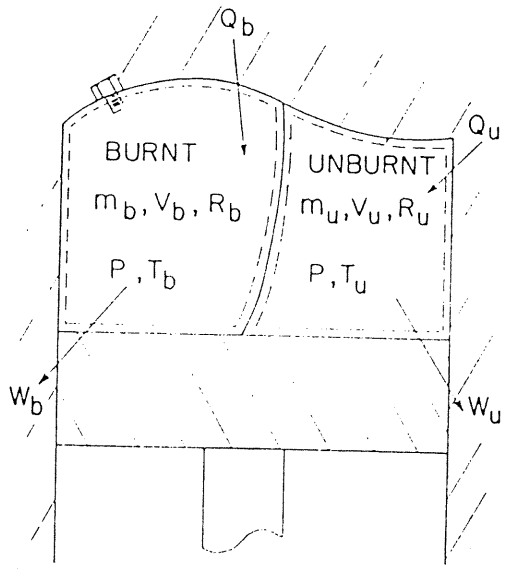

Fig. (1) Schematic Diagram of the Two Zone Model Assumed [8].

The energy equation for the unburnt zone is:

$$dQ_u = d(M_u C v_u T_u) + PdV_u - h_u dM_u \quad (2)$$

where dQ_u is the net external heat transfer from the unburnt zone.

The energy equation for the burnt zone is:

$$dQ_b = d(M_b C v_b T_b) + PdV_b + h_u dM_u \quad (3)$$

where dQ_b is the effective burnt zone heat transfer that includes the energy release due to the combustion of the fuel in dM_u and the heat transfer through the burnt zone walls. The combustion energy release rate due to the burning of the fuel can be derived from an energy release pattern which needs to be defined. From the analysis of mass of experimental data using mainly methane as the fuel an effective formulation for the mass burning rate can be made that is adequate for modelling knock [10].

The combustion energy release takes place over a certain combustion period $\Delta\theta_c$ that starts at θ_s, from just beyond the instant of spark timing after an ignition lag time when energy just starts to be released due to flame kernel development, and ends at θ_e as a result of the ending of flame propagation. The area enclosed by the resulting energy release diagram would represent the total effective energy released by combustion. The examination of a very large number of such diagrams for a wide range of operating conditions indicated that the *shape* of these diagrams tends to be similar. A very simple approach may consider such diagrams to approximate to triangles. The base is the corresponding combustion period and the area is the known total energy release.

The combustion duration in a spark ignited engine can be estimated in principle by resorting to the appropriate modelling of turbulent flame propagation within the confines of the changing engine cylinder. This is not an easy matter and the reliability of the outcome of such modelling remains at present to be uncertain. Accordingly, merely for the purpose of knock modelling, a simpler empirically based approach is proposed. The variation of combustion duration with equivalence ratio is found to have a trend similar to that shown typically in Figure (2). Moreover, the ignition limits which correspond to extremely long combustion periods, can be established experimentally or estimated for any specific engine [10]. The minimum combustion period can also either be measured experimentally or estimated [11]. Therefore, appropriate combustion period correlations can be formulated for any engine operating conditions. As an example, we used the following formula:

$$\Delta\theta_c = A\theta^x + B\theta^y \quad (4)$$

where $$x = (\phi_{min} - \phi)/(\phi - \phi_L)^{1/2} \quad (5)$$

and $$y = -(\phi_{min} - \phi)/(\phi_R - \phi)^{1/2} \quad (6)$$

$\Delta\theta_c$ is the combustion duration in degrees for an equivalence ratio of ϕ. The lean and rich operational limits equivalence ratio are ϕ_L and ϕ_R respectively. The equivalence ratio for minimum combustion time is ϕ_{min} which is usually around stoichiometric ($\phi_{min} \approx 1.0$). A and B are constants that can be derived in terms of ϕ. Since the combustion period becomes excessively long as the limits of mixture operation are approached and reaches a minimum around the stoichiometric mixture, the following two equations apply:

$$A + B = \Delta\theta_{c,min} \quad (7)$$

and

$$A/B = [(\phi_{min} - \phi_L)/(\phi_R - \phi_{min})]^{1/2} \quad (8)$$

where $\Delta\theta_{c,min}$ is the minimum combustion duration which is usually encountered around the stoichiometric region.

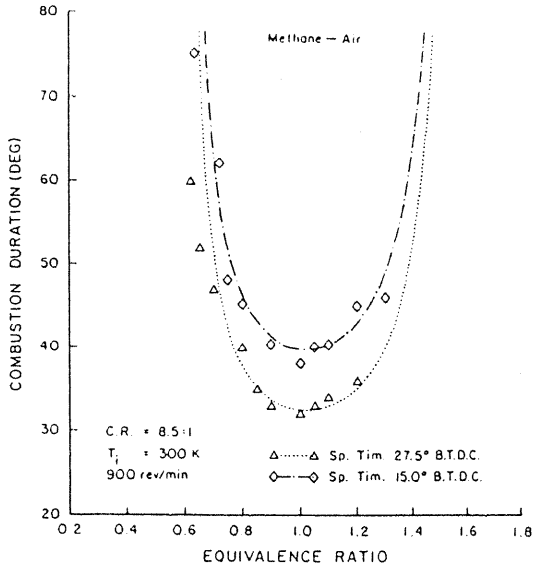

Fig. (2) Fitted values of the Combustion Duration According to Equation (4) with Equivalence Ratio for Two Spark Timings; the Experimental Data are also Shown.

Several functions have been suggested in the literature to represent the mass burning rate in spark ignition engines. For example, triangular, sine and Wiebe type functions have been used. The mass of data obtained experimentally when methane is the fuel over a very wide range of operating conditions that included variations in compression ratio, intake temperature, equivalence ratio, diluent addition and spark timing, as shown in Figure (3), followed approximately a triangular format [11].

The solution of the set of the relevant simultaneous equations employing numerical methods yields values of all the main properties of the cylinder charge and of the two zones and their variations with time. From a knowledge of the cylinder pressure variations with volume changes, the corresponding indicated power and output efficiency could be evaluated.

A number of schemes varying in complexity and detail can be employed to represent the oxidation of fuel within the end gas region. In this investigation, a somewhat brief reaction scheme, similar to that used by Karim and Zhaoda [12] modelled the preignition and combustion reactions of methane-air systems. It involved some 32 elementary reaction steps and 14 reactive species. Other fuels and schemes could be similarly considered.

As a result of these calculations, the temperature, pressure, volume and density of the reactive region of the end gas become known as a function of time throughout the

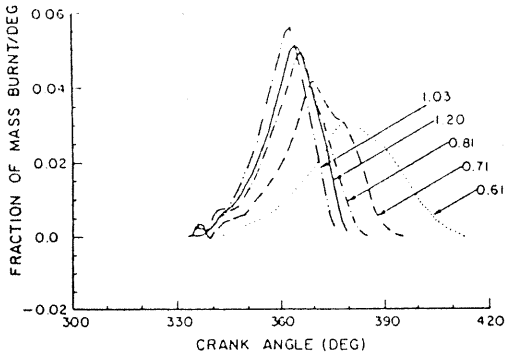

Fig. (3) Typical Variations of the the Rate Mass Burnt Change with Crank Angle Over the Combustion Period for a Range of Equivalence Ratios in a CFR Engine [10].

combustion period while turbulent flame propagation is proceeding. Hence, the net rate of production and consumption of each of the species (i) will be a function of the rates of all the reaction steps (j) involved and that proceeding simultaneously:

$$-\rho \frac{dx_i}{dt} = \sum_{j=1}^{j=32} (\alpha_{ijf} - \alpha_{ijb}) (R_{jf} - R_{jb}) \qquad (9)$$

where R_f and R_b are the forward and backward reaction rates, respectively. The set of simultaneous non-linear first order equations were solved numerically.

In the modelling of knock the reaction activity of the end gas is monitored using the approach described right from the time of spark ignition or even earlier during compression where necessary. This is carried out for each time increment while

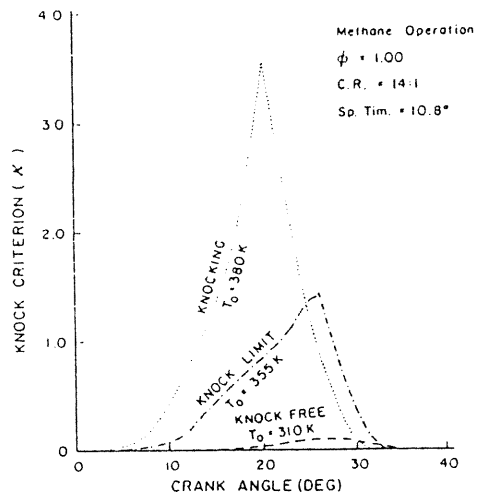

Fig. (4) Calculated Variations of the Knock Criterion $\mathcal{K}$ with Crank Angle for Three Cases Involving Knock Free, Knock Limit and Heavy Knocking Operation for a Stoichiometric Mixture of Methane-Air and Three Different Initial Temperatures.

accounting for the local temperature, pressure and volume of the end gas throughout, right up to the point of the total consumption of the unburnt charge by the propagating flame at the end of the combustion period. If during the whole process of combustion due to flame propagation, the concentrations of products or the reactants in the unburnt end gas region change significantly as a result of substantial reaction activity, then autoignition of the end gas may take place.

At each time interval the reaction rates and the associated changes in concentrations the end gas were calculated at the predicted T_{un} and P values. The maximum temperature change of the end gas zone due to these reactions was evaluated on the basis of an adiabatic constant pressure process. If this resulting calculated temperature change was significant, then it was used as the dT_{un} for calculating the reaction activity within the next time interval, instead of the value derived from the simple two-zone combustion progression model. It was found that when operating conditions were far from those producing knock, the changes in the unburnt gas temperature due to reaction activity expectedly were negligible compared to those of the energy release due to combustion and piston motion. But, when operating conditions produced significant end gas reaction activity, this calculated T_{un} value increased quickly speeding up the preignition reactions and bringing about autoignition earlier and with greater intensity than had the reaction activity been based on the value of temperature calculated from the two zone model.

A DIMENSIONLESS KNOCK CRITERION ($\mathcal{K}$)

The reactions of the end gas must release sufficient amount of energy to lead to autoignition and produce knock in engines. In addition to satisfying the conditions for the onset of autoignition within the end gas region, a sufficient amount of energy release and hence end gas must be involved.

A criterion for establishing whether knock is encountered in spark ignition engines must consider the total energy released

within the end gas due to autoignition reaction activity per unit of the corresponding instantaneous volume. Such a specific energy release needs to be compared for any engine, fuel and operating conditions to the corresponding total energy release that would take place normally due to regular flame propagation. The latter needs to be related to the total cylinder size and its volume. A dimensionless knock criterion ($\mathcal{K}$) can thus be defined as a ratio of the following two relative energy releases variation during the course of the combustion process:

$$\text{Knock Criterion } (\mathcal{K}) = \frac{\text{Energy of End Gas Reactions/(Volume)}_t}{\text{Energy of Combustion/(Volume)}_o} \quad (10)$$

where the numerator represents the total energy released by the preignition reactions activity of the end gas per unit instantaneous cylinder volume, while the denominator is the total energy that can be released normally through flame propagation per unit of initial cylinder capacity.

Since the spark timing is usually set such that much of the combustion process takes place in the vicinity of the top dead centre position so as to achieve optimum efficiency and power, then V_o/V_t can be approximated to $(r - 1)$ where r is the compression ratio. Therefore, the value of this knock criterion $\mathcal{K}$ at any time t may be represented by the following simplified form:

$$\mathcal{K} = \frac{(C_o - C_t)\, M_t\, (r - 1)}{C_o M_o} \quad (11)$$

The value of $(C_o - C_t)$ is obtained from the chemical kinetic calculations described earlier and would represent the difference due to chemical reaction activity between the initial fuel concentrations within the end gas and that at a time t prior to the incidence of autoignition. M_t is the mass of the unburnt zone which is the end gas region at any instant of time, t. This ratio also can be viewed to represent the pressure change due to the preignition reaction activity of the charging end gas relative to the Mean Effective Combustion Pressure.

It is clearly evident when there is neglible end gas reaction activity, no autoignition will take place within the combustion period (i.e. $C_o \approx C_t$ throughout) and the factor will remain negligibly small. However, when autoignition will take place, a significant size of the end gas will be involved, making the value of $\mathcal{K}$ unacceptably large. It is to be shown that the value of $\mathcal{K}$ for any operating conditions reaches a maximum value before the end of combustion and its value can be used to establish whether knock is to take place or not and its likely intensity.

RESULTS AND DISCUSSIONS

Figure (4) shows how the calculated value of the dimensionless knock criterion $\mathcal{K}$ varies over the whole combustion period for the three typical conditions when knock free, borderline knock and heavy knock operations were experimentally identified. It can be seen that for the case that was reported to have been knock free, the value of the calculated parameter $\mathcal{K}$ remained throughout very small. The case with heavy knocking associated with a high intake temperature preheating, in contrast produced very high $\mathcal{K}$ values. The case with borderline knock, had lower $\mathcal{K}$ values with the maximum value around 1.45.

It is evident throughout that as flame propagation proceeds, the unburnt gas temperature, T_{un}, increases bringing about increasing preignition reaction activity and contributing to increasing the values of $\mathcal{K}$. However, as the flame propagates, the size of the end gas region and hence the total energy released by the remaining unconsumed charge decreases rapidly to an eventual value of zero when flame propagation and the consumption of the entire end gas have been completed. The threshold of the incidence of mild knocking in this CFR engine is associated with a maximum value of around 1.45. Figure (5) shows the variations in the calculated dimensionless knock criterion $\mathcal{K}$ over the whole combustion period for the engine when only the equivalence ratio is changed while other operating conditions are maintained throughout constant. It was established experimentally that light knock operation takes place for these conditions at around the stoichiometric value. Intense knocking was encountered with an equivalence ratio of 1.10. It can be seen that the $\mathcal{K}$ values for the non-knocking operating conditions were below 1.45, while the peak values of $\mathcal{K}$ for the case of $\phi = 1.10$, was much in excess of 1.45.

Similarly, increasing the intake temperature for a specific set of operating conditions shortened the combustion period, due to faster flame propagation, while increasing the $\mathcal{K}$ value due to much increased reaction activity. The peak value of $\mathcal{K}$ then appears again to be around 1.45. Intense knock produced correspondingly higher peak values of $\mathcal{K}$. Another example that involves only variation in compression ratio so as to proceed from non-knocking to borderline knocking at 13:1 and to intense knock at higher values of compression ratio, is shown in Figure (6). It can be seen that increasing the compression ratio increases the peak value of the calculated parameter $\mathcal{K}$ very drastically. The operating conditions that are associated with very light borderline knocking has a peak value of $\mathcal{K}$ that is again around 1.45.

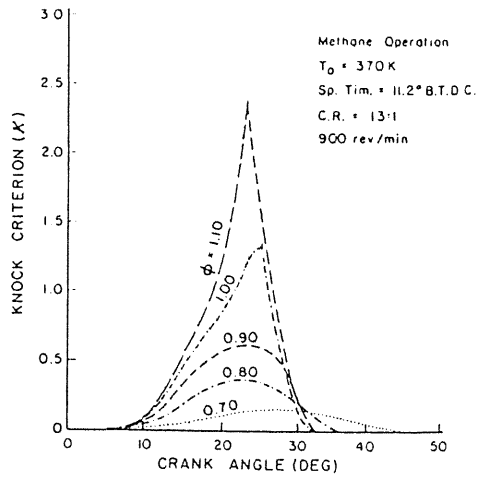

Fig. (5) Variation of the Calculated Knock Criterion $\mathcal{K}$ with Crank Angle for Different Equivalence Ratio Values; Heavy Knock is Associated with $\phi = 1.10$ [4].

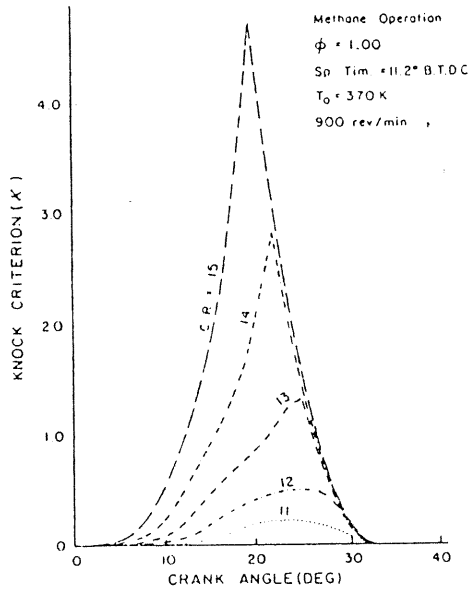

Fig (6) Variation of the Calculated Knock Criterion with Crank Angle for a Stoichiometric Methane for a Mixture at Different Compression Ratios; Knocking is Associated with C.R.s of 14 and 15:1 [4].

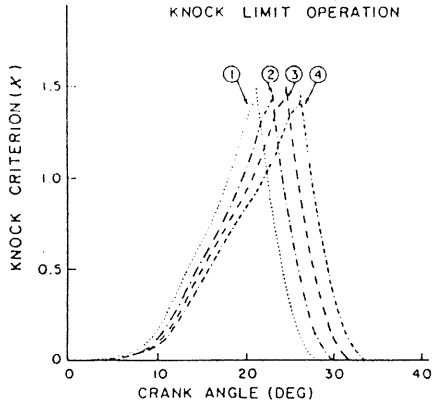

Fig (7) Variation of the Calculated Knock Criterion $\mathcal{K}$ with Crank Angle for $\phi = 1.0$ for Four Different Operating Conditions at which Knock Limited Operation with Methane was Encountered:

(1) T_o=415K, r=11:1, θ_s=12.5°; (2) T_o=391K, r=12:1, θ_s=11.8°; (3) T_o=372K, r=13:1, θ_s=11.2; (4) T_o=355K, r=14:1, θ=10.8°.

The variations in the value of $\mathcal{K}$ over the combustion period for a range of operating conditions where only the spark timing is advanced so as to proceed from non-knocking conditions right up to heavy knocking was also considered. The spark timing advance that produced very light knocking was associated with a maximum $\mathcal{K}$ value of around 1.45.

It appears from examining operating conditions in a CFR spark ignited methane fuelled engine that those conditions that will not produce a calculated value of $\mathcal{K}$ in excess of just over 1.0 over the whole combustion period will be associated with knock free operation. Operating conditions associated with higher peak values of $\mathcal{K}$ produce knocking. The more intense is the knocking, the higher is the peak value of $\mathcal{K}$. In order to avoid the onset of knock, operating conditions should be chosen such that the peak value of $\mathcal{K}$ remains not much greater. For example, Figure (7) shows four different operating conditions producing the same calculated peak value of $\mathcal{K}$ of 1.45 and correspond with experimentally observed borderline knock in the CFR engine.

CONCLUSIONS

The simple two-zone model described can generate important performance parameters such as the pressure ~ time development record and hence power output for a spark ignited engine fuelled with methane.

The model can be used to test for the occurrence of knock for any set of operating conditions while employing detailed reaction kinetics for the end gas region. The corresponding calculated value of the dimensionless knock criterion $\mathcal{K}$ developed can provide an indication of the intensity of the resulting knock when it occurs. Good agreement with experimental data has been demonstrated. For the engine tested, knock free limit was found to be associated with a maximum value of $\mathcal{K}$ that is less than 1.45.

ACKNOWLEDGEMENTS

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