

# Knock in Dual Fuel Engines

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## ABSTRACT

Description is given of an approach for predicting the onset of knock in compression ignition engines of the direct injection type when operating on pure gaseous fuels and their mixtures that may include methane, ethane, propane and hydrogen. The associated variations with time of engine performance parameters such as the energy release rate, cylinder pressure, mean charge temperature and power output can be established also. This is achieved by modelling in detail the chemical reaction rates of the gaseous fuel and heat transfer to the walls, both during compression and subsequently during diesel fuel pilot ignition and combustion to establish whether autoignition and hence knock will take place.

## NOTATION

$A_s$	Surface area for heat transfer
$C_v$	Specific heat at constant volume
$M$	Mass
$Q_p$	Energy release rate by pilot
$R^p$	Reaction rate or Universal gas constant
$T$	Temperature
$t$	time
$U_f$	Internal energy of formation
$V$	Volume
$x$	Concentration
$\alpha$	Stoichiometric coefficient
$\rho$	Density

## Subscripts

b	backward reaction
f	forward reaction
i	species 'i'
j	reaction step 'j'
w	wall

## INTRODUCTION

One of the problems associated with the conversion of a direct injection diesel engine to dual fuel operation is that at high load operation, the maximum power output is limited by the onset of knock which involves exceedingly rapid rates of energy release. It is due to an autoignition phenomenon dominated by the chemical kinetic reactions of

the premixed fuel-air system. It is strongly dependent on the type of gaseous fuel used and other working conditions such as intake temperature.

A great deal of research into the knock phenomena in dual fuel engines has been carried out over the years [e.g. 1, 2, 3, 4]. Karim and Klat [5] investigated experimentally the effects of changes in various operating parameters such as intake temperature and the quantity and quality of the pilot liquid fuel on the knock performance limits, while using various gaseous fuels (propane, methane and hydrogen) and their blends. Their findings supported the view that the knock observed in a typical dual fuel engine is mainly caused by the autoignition of the gaseous fuel-air mixture in the neighbourhood of the ignition centres arising from the small pilot liquid fuel sprays.

Karim and Zhaoda [6] provided a quasi-two zone model for simulating the phenomenon of autoignition and knock through improved modelling of the chemical reaction rates of the gaseous fuel during compression and subsequently following pilot ignition. The calculated results were based mainly on methane and the contribution of pilot diesel injection to the energy release of the engine was considered. Karim and Liu [7] developed this predictive model further to include a more detailed chemical kinetic mechanism of higher hydrocarbon oxidation for fuels up through C3, such as propane, ethylene and their blends.

In the present contribution, the effects of the admission of propane, methane, hydrogen and their mixtures on the knock characteristics and operation of a dual fuel engine are examined through modelling in detail the chemical reaction activity of the preignition and subsequent combustion processes. Predicted values are then compared with the corresponding experimental performance.

## The Combustion Process in Dual Fuel Engines

The combustion process in a typical dual fuel engine, depends both on the spray and ignition characteristics of the diesel pilot fuel and on the type of the gaseous fuel being used and its overall concentrations in the cylinder charge. There are in principle three modes of combustion in such engines. The first, when a very lean gaseous fuel-air mixture is admitted, will result in only the

pilot fuel and the gaseous fuel within the spray zone burning. The flames from the various pilot ignition sources cannot propagate throughout the very lean surrounding gaseous fuel-air mixture. This incomplete combustion leads to decreased engine efficiency, lower power output and increased emissions of the unburnt fuel and carbon monoxide. A further increase in the gaseous fuel concentration in the cylinder charge to the level associated with the corresponding local effective flame propagation limit of the gaseous fuel, will allow the flames to progress well into the mixture outside the pilot fuel spray region. In time, the combustion zone will extend into the whole mixture. This mode of combustion is associated with faster overall combustion rates and a greater energy release throughout, resulting in high power outputs and efficiency with favourable exhaust emissions.

The continued increase of the gaseous fuel concentration or intake temperature can lead eventually to the onset of autoignition and knock. The preignition reactions of the gaseous fuel around the pilot fuel region become so active that once the pilot fuel ignites, combustion takes place both inside and outside the pilot fuel spray zone. The pilot and the gaseous fuels can then burn so rapidly and almost simultaneously as to result in extremely high energy release rates and a fast pressure rise. Therefore, the knock phenomenon observed in dual fuel engines, which is of an autoignition nature of the gaseous fuel-air mixture, especially in the neighbourhood of the pilot fuel ignition centres, is essentially related to the autoignition of the same mixture under motored operation.

### A Simple Analytical Model for Knock

A quasi-two zone analytical model based on that described by Karim and Zhaoda [6] was developed to establish the onset of autoignition and knock. In this model, the entire gaseous fuel-air charge in the cylinder is treated as the main zone subjected to changes in pressure and temperature with time due to piston motion and preignition and combustion reactions. A subsidiary zone accounts for the contribution of the pilot fuel to the autoignition processes. During the stages of compression, combustion and expansion, full chemical reaction kinetics were employed to predict in detail changes in composition and the associated properties due to the reactions of the gaseous fuel-air charge.

The kinetic scheme employed in the present analysis could describe the preignition and combustion reactions of a gaseous fuel such as propane, methane or hydrogen within the range of dual fuel operations that involve generally lean mixtures at relatively high temperature and pressure conditions. The chemical reaction mechanism employed was based on those recommended by Karim and Liu [7], Warnatz [8] and Westbrook [9]. The scheme employed in the present work consisted of 138 elementary reaction steps and 32 chemical species. The corresponding thermo-chemical data were obtained mainly from JANAF tables [10].

The net rate of change in the concentration of each species ( $x_i$ ) will be a function of the rates ( $R_{if}$ ,  $R_{ib}$ ) of all the reaction steps ( $j$ ) involved that are proceeding simultaneously and is given by a general relationship of the form:

$$-\rho \frac{dx_i}{dt} = \sum_{j=1}^{j=138} (\alpha_{if} - \alpha_{ib}) (R_{if} - R_{ib}) \quad (1)$$

The energy equation for the homogeneous reacting system assumed to be an ideal gas prior to pilot ignition becomes:

$$\sum_{i=1}^{i=32} x_i R T \frac{dV(\theta)}{V(\theta)} + \sum_{i=1}^{i=32} \left( \int_{T_0}^T C_{v,i} dT + \Delta U_{f,i} \right) \frac{dx_i}{dt} + x_i C_{v,i} \frac{dT}{dt} = \lambda (T - T_w) \frac{A_s}{M} \quad (2)$$

Thus, the simultaneous set of equations of (1), one for each species, and the energy equation (2), result in a set of non-linear first order simultaneous equations which were solved numerically. Other properties such as pressure, energy release rate, etc., can be derived once the concentrations and temperature have been determined.

A simple yet effective approach was developed to account for the presence of the pilot in the autoignition processes of the fuel-air mixture in the cylinder. This approach assumes that the pilot acts on ignition merely as a source of thermal energy for the gaseous fuel-air charge and ignores the complexities of any chemical interaction. Accordingly, an energy release rate for the pilot fuel during its ignition and subsequent combustion can be assumed and used based on actual experimental records of diesel engine operation. Hence, energy equation (2) is then modified to the following:

$$\sum_{i=1}^{i=32} x_i R T \frac{dV(\theta)}{V(\theta)} + \sum_{i=1}^{i=32} \left( \int_{T_0}^T C_{v,i} dT + \Delta U_{f,i} \right) \frac{dx_i}{dt} + x_i C_{v,i} \frac{dT}{dt} = \lambda (T - T_w) \frac{A_s}{M} + \dot{Q}_p \quad (3)$$

Where  $\dot{Q}_p$  is the rate of energy release due to the combustion of the pilot.

The ignition delay value of the pilot could be also established either experimentally for the specific engine and fuels employed or using one of the empirically derived formulae available in the literature. For consideration of the heat transfer from the charge, the mean wall temperature ( $T_w$ ) was assumed to remain constant, while convective and radiation heat transfer accounted for using a suitable formulation recommended by Annand [11], following analysis of a range of experimental data in engines.

### Results and Discussion

The reactivity of the gaseous fuel-air mixture varies widely with the type of fuel and its overall concentration in the cylinder charge. Fig.1 shows the addition of hydrogen to the engine intake air, in the absence of pilot fuel injection, reduces the maximum temperature level of the charge only relatively little as the equivalence ratio is increased. This is mainly because of the slight relative lowering of the specific heat of the mixture with increased hydrogen admission. It is in contrast to the marked decrease in the values of the maximum charge temperature observed with the addition of methane or propane. With propane addition, the lowering of the peak value of the charge temperature was especially large being around 100 K for the stoichiometric mixture. This is consistent with the trends observed for a dual fuel

engine that with propane addition the ignition delay is longer than that observed with hydrogen or methane additions, despite the fact that propane is considered to be relatively more reactive than either hydrogen or methane under the same conditions [2]. However, hydrogen in comparison is relatively inactive during the preignition reaction process. As shown in Fig.2, the net maximum energy release rate is increased almost linearly with the increased admission of hydrogen to the cylinder charge. This is because the reactivity of the mixture is improved with the increase of the overall concentration of the hydrogen, while the effective mixture temperature does not change significantly with hydrogen admission.

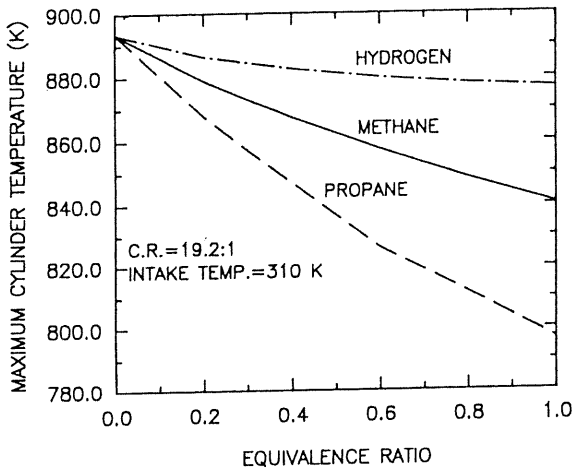


Fig.1 The Variation of the Maximum Cylinder Temperature with Equi. Ratio for Propane, Methane and Hydrogen

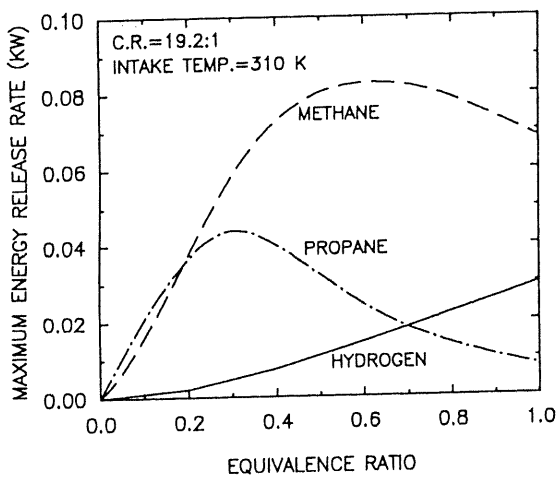


Fig.2 The Variation of Max. Energy Release Rates with Equivalence Ratio for Propane, Methane and Hydrogen

With methane admission the net energy release rates of methane and propane show markedly different trends from that observed with hydrogen admission. The peak values of the calculated energy release rate display a maximum value that is located well onto the lean side of the stoichiometric ratio, as a result of the decreased effective mixture temperature with methane and propane admission. It can be seen that for any equivalence ratio, the maximum value of the energy release associated with hydrogen admission is lower than those obtained with methane or propane admission, even though its maximum charge

temperature is higher than those values observed with methane or propane admission. The preignition reactivity of hydrogen in the engine, which shows distinctly different characteristics from those of the other fuels, tends to be low but is strengthened with the increase of hydrogen concentration in the cylinder charge. Hence, the knock characteristics of dual fuel engines can vary significantly with the gaseous fuel used.

The variations of pressure and temperature in the operation of a typical dual fuel engine are very important indicators that show whether knock is encountered or not for any fuel system under a specified set of operating conditions. The calculated rates of pressure and temperature rise increase markedly with increasing the methane concentrations in the cylinder charge. Following the ignition and combustion of a small amount of pilot fuel, relatively high temperatures are produced locally from the ignition and combustion of the methane. The onset of knock in the calculated model is associated with the production of unacceptably very high values of rates of charge pressure and temperature rises as a result of the rapid combustion of the gaseous fuel. On this basis, the predicted values for the onset of knock were generally in good agreement with the corresponding experimental values [5].

Fig.3 shows logarithmically the variation of the calculated energy release rates with time for a number of cases involving mixtures of different equivalence ratios, while employing a fixed pilot quantity. The variation with time of the energy released by the small quantity of the pilot fuel tends to be smooth and is associated with low rates. The energy released by the combustion of the lean mixture of methane fuel is relatively low throughout and extends well down into the expansion stage. With an increase of the methane concentration in the cylinder mixture, the start of the preignition reactions is advanced and the reaction time to achieve maximum energy release rate is greatly shortened. Much more energy is released from the rapid combustion of the methane. The continued increase in methane admission leads eventually to the onset of intense knocking with an equivalence ratio of 0.70, immediately following pilot fuel ignition.

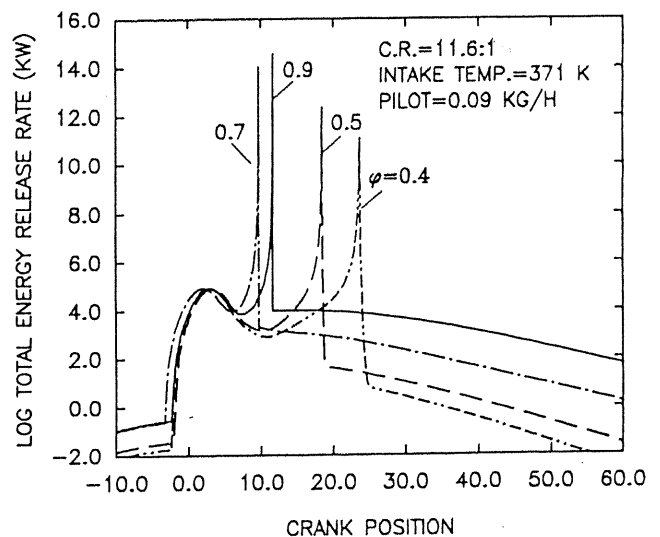


Fig.3 The Variation of Log Energy Release Rates with Crank Position Over a Range of Equivalence Ratio for Methane, Admission. The Knock Experimental Range: 0.72–0.92 (5)

Raising the intake temperature will allow combustion to be sustained at even leaner mixtures and will alter the boundaries of the knocking region of the dual fuel engine. Fig.4 shows the variations of the calculated and corresponding experimental regions for knocking operation with propane, methane and hydrogen over a wide range of intake mixture temperature. These regions shown on total equivalence ratio basis (i.e. including the pilot) are widened significantly with the increase in intake temperature and are strongly dependent on the type of fuel being used. The knock region for methane varied little with the changes in intake temperature. However, for propane and hydrogen operation they are widened significantly with the increase of intake temperature and extend into lower intake temperatures where the onset of knock is associated with relatively rich mixtures of the propane and hydrogen. The predicted values of the knocking regions for methane and propane admission can be seen to agree well with the experimental values. However, for operation with hydrogen, good agreement appears to be only for relatively high intake temperatures, indicating that the autoignition model may not necessarily represent well the onset of knock with hydrogen at relatively low intake temperatures and with mixtures of less lean equivalence ratios.

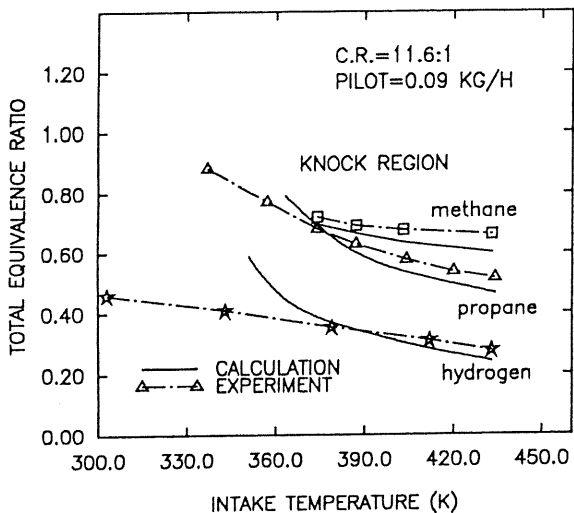


Fig.4 The Variations of Predicted and Experimental Knock Range with Intake Temperatures for Propane, Methane and Hydrogen Admission

The quasi-two zone model employed assumes that autoignition is the outcome of the acceleration of chemical reaction rates of the gaseous fuel-air mixture. Hence, the calculated knocking regions for propane, methane and hydrogen agree well with experiment at high intake temperatures. However, the analysis of preignition reactions of hydrogen showed that it tends to resist the tendency to autoignition within the time available for low intake temperature operation. Accordingly, the experimentally reported onset of knock with hydrogen at low intake temperature may not be due to autoignition but is the result of the very high rates of energy release arising from the very rapid flame propagation to be noted with the increased concentration of hydrogen in the cylinder mixture. Thus, it can be seen that great care is needed when operating dual fuel engines on hydrogen because of the relatively wider knocking region associated with such operation. Fig.5 further shows that the power output of a dual fuel engine operating on hydrogen is markedly limited by the increase in the intake temperature and the onset of knocking. The

predicted limits for power output are in good agreement with the corresponding experimental results at relatively high intake temperatures but display substantial deviations from the experimental values at relatively low intake temperatures. Since hydrogen has different knocking characteristics from those observed with different gaseous fuels, the present calculated results are in agreement with the corresponding experimental performance [5], which shows that the knock limited power output with hydrogen is reduced linearly with the increase in intake temperature. This is in contrast to propane and methane admissions where the knock limited power output is shown to be reduced logarithmically with the inverse of the absolute value of the intake temperature, being consistent with the autoignition origin of such knocking (5).

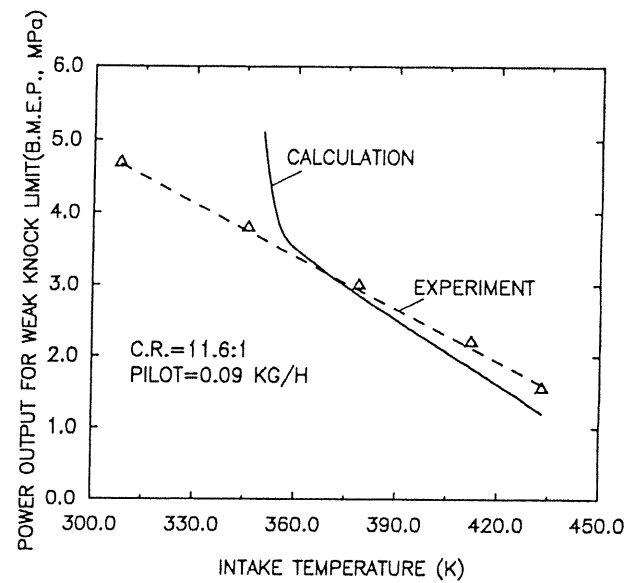


Fig.5 The Variations of the Calculated and Experimental Power Output for Knock Limit with Intake Temperature for Hydrogen Admission

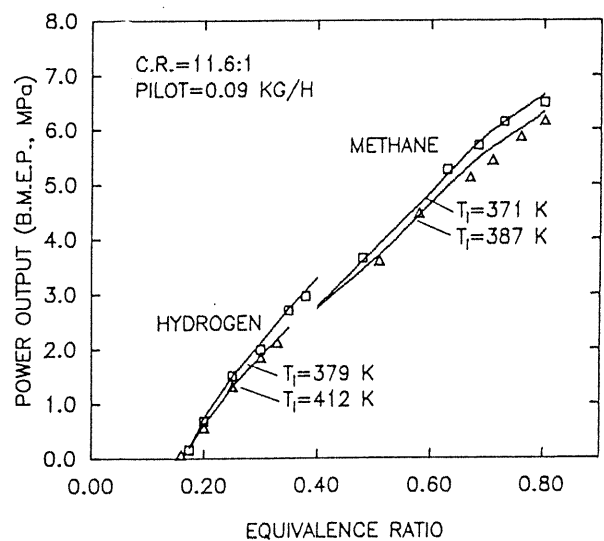


Fig.6 The Variation of Predicted and Experimental Power Output with Equivalence Ratio over a Range of Intake Temperature for Methane and Hydrogen Admission

Fig.6 shows the variations of calculated and experimental power output with the total equivalence ratio

for a range of heated intake temperature values at a constant pilot quantity. It can be seen that the power output of a typical dual fuel engine is increased with increasing the gaseous fuel content of the cylinder charge but it is decreased with the raising of intake temperature, mainly as a result of the reduction of the charge density. The power output with methane admission is significantly higher than those with hydrogen admission, because of the knock limitation of hydrogen operation. The calculated power output shows on the whole good agreement with the corresponding experimental values for both fuels.

## Conclusions

The incidence of knock in a dual fuel engine is strongly dependent on the type of gaseous fuel being used. The regions for knocking operation with hydrogen admission are wider than those encountered with methane and propane. The calculated knocking regions for propane, methane and hydrogen agree well with the corresponding experimental values at high intake temperatures, but the operation with hydrogen displays substantial deviations from the experimental values at relatively low intake temperatures.

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