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Knock prediction for dual fuel engines by using a simplified combustion model*

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Abstract: The present work used a methane-air mixture chemical kinetics scheme consisting of 119 elementary reaction steps and 41 chemical species to develop a simplified combustion model for prediction of the knock in dual fuel engines. Calculated values by the model for natural gas operation showed good agreement with corresponding experimental values over a broad range of operating conditions.

Key words: Dual fuel engines, Combustion model, Knock prediction
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INTRODUCTION

Due to dwindling fuel oil reserves and the desire for reduced pollutant emissions, natural gas, which is dominantly composed of methane, has been now widely used as an alternative fuel in internal combustion engines. A conventional diesel engine can be converted without excessive increase in cost to a dual fuel engine, in which the combustible methane-air mixture is ignited by a small quantity of diesel fuel (pilot). As a result, the combustion pollutants can be reduced to a relatively low level. However, it can lead to knock when the compression ratio is high. In order to decrease knock in dual fuel engines, a fundamental understanding of the detailed reaction mechanism involved is required so that this knowledge can be applied to increase the knock resistance of dual fuel engines.

Although many researchers have pursued studies on knock, research on the knock chemistry kinetics of methane-air mixture in dual fuel engines is still in a developmental stage(Karim, 1988). With the development of computer simulation technology, chemical kinetics modeling has been widely used to predict the performance and emission of dual fuel engines(Fei, 1993).

As the reaction rates employed in the combustion model strongly affect the predicted performance, it is better to validate the reaction rates against reliable experiment results of methane auto-ignition under relevant conditions. Spadachini *et al*. (1994) and Petersen *et al*. (1999) did some research work on methane auto-ignition and published experimental results helpful in making combustion simulation more reliable. On the basis of the experimental results, a simplified reaction mechanism consisting of 11 steps was derived specifically for knock prediction. Good agreement was found between numerical predictions and experimental results.

COMBUSTION MODELS FOR DUAL FUEL ENGINE

1. A model with detailed reaction mechanism

For a dual fuel engine, the gaseous fuel air charge in the cylinder is the main reaction zone and subjected to change in pressure and temperature with time by piston motion, pre-ignition and combustion reactions.

To simplify the analysis, it is assumed that all components of the mixture behave as ideal gases considered as at equilibrium state corresponding to the instantaneous temperature and

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pressure of the system. A detailed chemical kinetics scheme consisting of 119 elementary reaction steps, and 41 chemical species are employed to describe the oxidation of the gaseous fuel from the start of compression to the end of the expansion process.

The energy equation for the whole mixture system in the model is given by:

$$P \cdot \mathrm{d}V + \mathrm{d}U = \mathrm{d}Q + \mathrm{d}Q_{\mathrm{d}} \qquad (1)$$

Where $\mathrm{d}U$ is the incremental rate of internal energy for the charge due to the changes in temperature and chemical reactions of the mixture, $\mathrm{d}Q$ is the incremental rate of heat transferred to the charge, and $\mathrm{d}Q_{\mathrm{d}}$ is the incremental rate of heat released by combustion of the diesel.

The incremental rate of the internal energy can be expressed as:

$$\mathrm{d}U = \sum_{i=1}^{41} \{[(\int_{T_0}^{T} C_{V_i}\,\mathrm{d}T + \Delta U_f)(\mathrm{d}X_i/\mathrm{d}t)] + X_i C_{V_i}(\mathrm{d}T/\mathrm{d}t)\} \qquad (2)$$

The first term of the above equation is the incremental rate of internal energy due to variation of the charge composition, and the second term is due to change of the charge temperature. The net rate of production for each species, $\mathrm{d}X_i/\mathrm{d}t$ can be obtained by:

$$\mathrm{d}X_i/\mathrm{d}t = \sum_{j=1}^{119}(\alpha_{ijp} - \alpha_{ijr})(R_{jf} - R_{jb})/\rho \qquad (3)$$

Where α_{ijp} is the stoichiometric coefficient of ith species appearing in the products of the jth reaction, while α_{ijr} is the stoichiometric coefficient of ith species appearing in the reactants of the jth reaction, R_{jf} is the forward reaction rate for the jth reaction, and R_{jb} is the backward reaction rate for the jth reaction.

Accordingly, the derivation of the mean charge temperature with time can be obtained as:

$$\mathrm{d}T/\mathrm{d}t = \{\mathrm{d}Q + \mathrm{d}Q_{\mathrm{d}} - \mathrm{d}W - \sum_{i=1}^{41}[(\int_{T_0}^{T} C_{V_i}\,\mathrm{d}T + \Delta U_f)(\mathrm{d}X_i/\mathrm{d}t)]\}/\sum_{i=1}^{41}(X_i C_{V_i}) \qquad (4)$$

Thus, the increment of temperature and a set of species concentrations at the end of the time can be calculated, and the pressure of the cylinder can also be obtained.

2. A simplified model for knock prediction

Accurate prediction of auto-ignition is critical for the study of natural gas combustion. Literature review revealed that shock-tube experiments on methane had been thoroughly investigated by Spadaccini *et al*.(1994), and Petersen *et al*.(1999). It can be seen that the end-gas equivalence of methane-air mixture in dual fuel engines falls in the range of measurements of Spadaccini *et al*., while the end-gas temperature (800K – 1200K) and the pressures (5×10^6 – 1.5×10^7 Pa) were closer to the measurements of Petersen *et al*.

The above mentioned chemical mechanism can be significantly simplified when it is applied to knock prediction in dual fuel engines where the end-gas equivalence ratios are low and the end-gas temperature ranges from 800K – 1200K. The reaction tendency and degree for a specified elementary reaction can be estimated through calculating enthalpy variation. By this sensitivity analysis, it was found that the 11 elementary reactions listed below are most important to auto-ignitions of methane-air mixtures in the temperature range below 1200K.

(1) $CH_4 + O_2 = CH_3 + HO_2$
(2) $CH_4 + HO_2 = H_2O_2 + CH_3$
(3) $CH_4 + OH = H_2O + CH_3$
(4) $CH_3 + O_2 = CH_3O + O$
(5) $CH_3 + OH = CH_2O + H_2$
(6) $CH_2O + OH = CHO + H_2O$
(7) $CH_2O + O = CHO + OH$
(8) $CHO + M = CO + H + M$
(9) $CHO + O_2 = CO + HO_2$
(10) $H_2O_2 + M = 2OH + M$
(11) $H + O_2 + M = HO_2 + M$

The most important initiation reaction is step (1), and step (2) begins to produce H_2O_2 and CH_3 as the HO_2 concentration builds up. When the CH_3 concentration is high enough, step (5) becomes important and creates CH_2O.

RESULTS AND DISCUSSIONS

To demonstrate some of the application of the model, predicted results relating to a 4 stroke single cylinder, D × S(108 mm × 150.4 mm), water-cooled, direct injection diesel test engine

are given in Figs. 1 and 2.

Fig. 1 shows the comparison between experimental and predicted results power produced with total equivalence ratio. Obviously, the power produced increased with the increased concentration of the gaseous fuel. As the assumptions, such as ideal gas, without leakage and so on, have been considered during the calculation, the prediction of power produced is a little higher than that obtained from experiment.

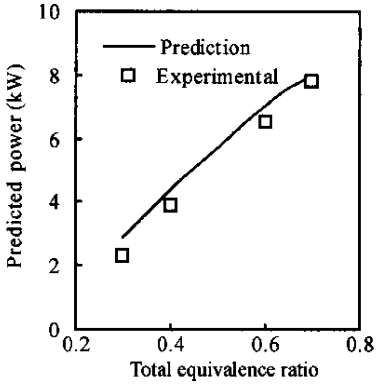

Fig. 1 Comparison between experimental and predicted results of power produced with total equivalence ratio

Fig. 2 shows predicted concentrations histories of CO using the 119-step mechanism and the 11-step reduced chemistry respectively. As expected, similar results were obtained using two reaction mechanisms.

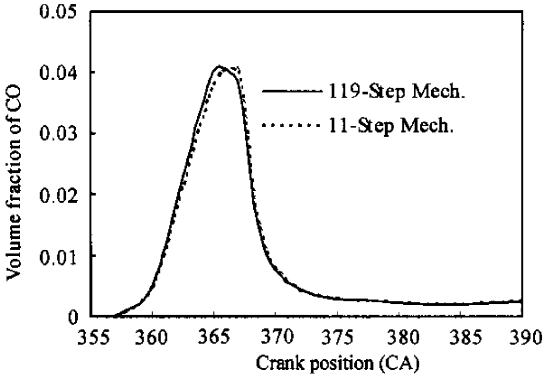

Fig. 2 Variations of carbon monoxide with crank position for different reaction mechanisms

For very lean fuel mixture operation (below the effective flammability limit), flame propagation does not occur. Within this range, it can be suggested that most of the carbon monoxide in the exhaust gases are produced from local partial oxidation of the methane air mixture due to the relatively slow reaction rates associated with low overall charge temperatures. On the other hand, during the expansion stroke, the mean temperature of the charge is gradually and continuously decreased resulting in partial oxidation of the remaining unreacted gaseous fuel. Therefore, for the fuel lean side, the carbon monoxide increases with increasing admission of the methane. However, a continuing increase in the concentration of the methane will lead to flame initiation and partial propagation, and a more complete oxidation of the mixture results in a corresponding decrease of carbon monoxide.

Experiments demonstrated that the dominant factors influencing knock occurrence for a specified compression ratio are T_{ic}, the mixture temperature after intake valves closed, and Φ, the equivalence ratios (Gebert, 1998). It was found that T_{ic} is higher than the mixture temperature in the intake process, which maybe caused by the heat transfer from the hot piston crown, cylinder liners and the hot residual gas from the previous cycles.

Typical results of experiments and numerical computations are plotted in Fig. 3 where the influence of T_{ic} on knock is shown. It is obvious that a higher gas temperature leads to an earlier and sharper temperature rise. Knock does not

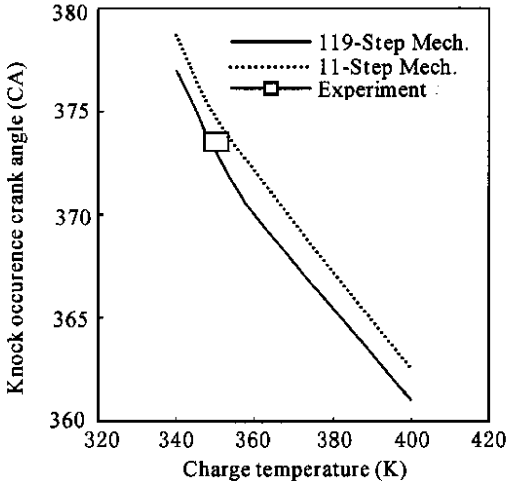

Fig. 3 Influence of charge temperature on knock with equivalence ratio $\Phi = 0.561$

occur when T_{ic} is low enough. This clearly demonstrates that the end-gas temperature plays an important role in preknock reactions in the end-gas zone.

The charge temperatures are increased with the increase of concentration of the methane in the cylinder charge. As higher equivalence ratio produces higher flame temperature and, as a result, creates higher surface temperature of the chamber wall, a higher Φ always leads to higher T_{ic}.

Fig.4 shows the variations of the calculated total energy release rate with crank position for different values of the equivalence ratios for methane admission. It can be seen from Fig.4, that prior to and during the premixed combustion phase of the pilot fuel, the energy released by the lean gaseous fuel air charge is relatively low. Higher rates of the combustion reactions within the gaseous fuel air mixture result in the much greater energy release rates observed immediately following ignition of the pilot fuel. Obviously, the maximum total energy release rate is increased with the increased concentration of the gaseous fuel.

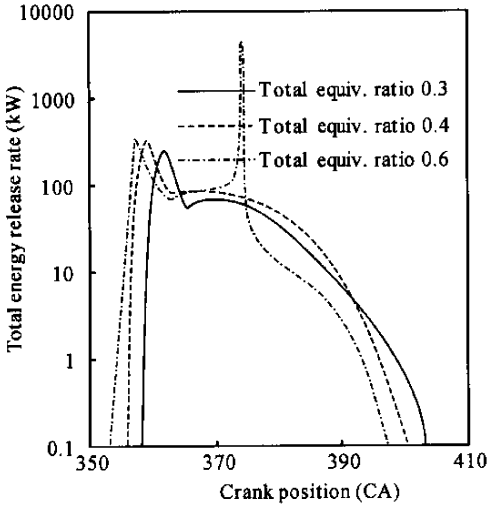

Fig.4 Variations of the calculated total energy release rate with crank position for different values of total equivalence ratio

From the predicted results above, the ability of the combustion model to predict the knock for dual fuel engine has been confirmed.

CONCLUSIONS

A full reaction mechanism, and an 11-step short mechanism have been developed for predicting knock occurrence in dual fuel engines. This work helps to identify the most important species and reactions that lead to knock. The effects of initial mixture temperature and total equivalence ratio were observed to be very effective in creating knocking conditions. Most predicted results showed good agreement with relevant experimental data.

As the reaction mechanism is reliable, it will be helpful to investigate how to increase knock resistance in dual fuel engines in practice. Therefore, the models described in this paper have significant value in theory and practice for dual fuel engine.

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