Analysis of Reaction Mechanism of DME/n-Butane Mixtures on Autoignition Characteristics of HCCI Combustion

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Abstract : Reaction mechanism for di-methyl ether (DME) and n-Butane mixture was analyzed on the autoignition characteristics of HCCI combustion. CHEMKIN-II was used as a solver and chemical-kinetics mechanism was made from Curran's DME and Kojima's n-Butane model. The addition of LPG was assumed by n-Butane. Mixing ratios of two fuels were firstly varied from pure DME to pure n-butane over intake temperature ranges from 300K to 460K in an increment of 20K in order to obtain the map of operating range. Investigations also concentrate on autoignition process of DME/n-Butane mixtures in the viewpoint of chemical reaction mechanism. The results show that its knock limit occurs at higher concentration of DME while higher n-Butane rates can be tolerated into operation zone. However, too much amount of n-Butane was the ignition suppressor, which means there was misfire.

Key words : Di-methyl ether, n-Butane, Reaction, Autoignition, Mixing ratio.

1. INTRODUCTION

Homogeneous charge compression ignition (HCCI) engine is named as the candidate of next generation internal combustion engine with the high efficiency of the CI engine and the very low emissions of the SI engine. Known benefits of HCCI are near-zero nitrogen oxides (NOx) and PM emissions. However, several items have to solve before its widespread production. Among these, controlling the rate of energy release and pressure-rise at high loads have been main problems [1]. There are many attempts made to overcome the problem of early ignition timing, which are making heterogeneous mixture or thermal stratification [2-3], adding cooled EGR [4], and mixing two different characteristics of fuels as high cetane and high octane number fuels [5], or vice versa. To approach that way, DME and LPG were used in this study as a fuel. DME has been taking much attraction as known the alternative of diesel fuel with smokeless combustion, low ignition temperature, superior properties of evaporation and available to produce from wide ranges of sources as natural gas, coal and vegetarian, etc. Besides these good characteristics, early ignition and short burn duration have been main obstacle and limits the wide production of DME fueled vehicles or the other applications. Therefore, adding LPG into DME as ignition inhibitor is the promising technology. Authors have conducted research on DME/n-Butane pre-mixture which shows that optimized mixing ratio has the potential to delay autoignition timing by reducing pressure riese rate (PRR). This is a continued work to understand better in the aspect of fundamental understanding for reaction mechanism since ignition of HCCI takes place by the dominance of chemical kinetics. The main objective of this study is to computationally investigate the autoignition mechanism of DME/n-Butane mixture in case of chemical kinetics. The “Contribution matrix to heat release” and “Absolute heat-release rate” of important elementary reactions are used for each fuel to identify the underlying mechanism by varying the mixing ratios.

2. COMPUTATIONAL APPROACH

2.1 Chemical-kinetics modeling setup

The computational investigations have been conducted using the SENKIN application of single-zone model of CHEMKIN II [6-7]. The single-zone model treats the in-cylinder charge as a single lumped mass with uniform composition and thermodynamic properties. Heat-transfer and blow-by effects were not included. Compression / expansion was modeled according to the standard slider-crank relationship, using the geometry and specifications of the single-cylinder HCCI engine shown in Table 1.

Table 1 Engine specification

Displacement (cc)	498
Bore (mm)	83
Stroke (mm)	92
Connecting rod length (mm)	145.8
Compression ratio	14.5:1
Number of valves	2
IVC (deg aTDC)	-132
EVO (deg aTDC)	125.4

2.2 Knock and misfire limits

For this study, the ringing correlation developed by Eng [8] is used to quantify the knock level:

$$Ringing\ Intensity \approx \frac{1}{2\gamma}\cdot\frac{\left(0.05\cdot\frac{dP}{dt,\max}\right)^2}{P_{\max}}\cdot\sqrt{\gamma RT_{\max}} \quad (1)$$

Eq.(1) shows that the ringing intensity is proportional to the square of the absolute maximum pressure-rise rate (in kPa/ms). 5MW/m^2 was chosen as the limit for allowable ringing. Refer to the maximum temperature of DME, the onset of misfire reactions can be judged when reaching the temperature below 1100K [9].

3. RESULTS

To get the map of operating zone of DME/n-Butane mixture in HCCI combustion, the effect of intake temperature for pressure rise rate (PRR) over various mixing ratio of DME was confirmed, which shows in the Fig.1. As can be seen, there was misfire at lower mixing ratio of DME at lower initial temperature. Lower PRR can be obtained at mixing ratio of .06 at 340K while higher

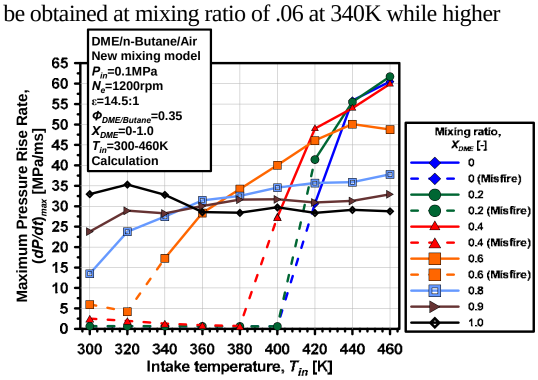

Fig. 1 PRR as a function of intake temperature over mixing ratios of DME.

mixing ratio of DME has operatable throughout the temperature range. Among them, X_{DME}=0.8 at 300K has the lowest PRR which was thought that it is possibility to expand high load limits with this way.

4. CONCLUSION

The increase of initial temperature results the increase of PRR over the mixing ratios. However, it has potential to reduce the PRR and expand high-load limit by optimizing the mixing ratio and intake temperature.

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