

AEC021

A Study on Combustion and Emission Characteristics of DME-LPG Dual Fuel in HCCI Engine

Narankhuu Jamsran¹, Ocktaeck Lim^{2,*}

¹ Graduate school of Mechanical Engineering, University of Ulsan, Ulsan, 689-749, Korea

² Department of Mechanical Engineering, University of Ulsan, Ulsan, 689-749, Korea

* Corresponding Author: otlim@ulsan.ac.kr, Tel.: +82522592852, Fax.: +82522591680

Abstract

This study was investigated the potential increase of engine power through the mixture of DME and LPG on HCCI combustion. The effects of mixing ratio of DME/LPG was confirmed experimentally in single cylinder diesel engine. To obtain higher engine output by changing the combustion phasing, intake temperature was varied. For the further analysis, numerical analysis were conducted for the detailed chemical kinetics using CHEMKIN-PRO. The results show that increase of the amount LPG reduces the LTHR and activates the HTHR which increases the in-cylinder pressure. Therefore, it has potential to raise the IMEP by appropriately changing the mixing ratio. Also, thermal efficiency increased to 51.2% as the mixing ratio of 0.6. Finally, engine out emissions as THC and CO were decreased by the change of mixing ratio. Numerical results agreed with experiment that the weakened LTO by the increase of n-Butane amount.

Keywords: Mixing ratio, Indicated mean effective pressure, Combustion phase.

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 (NO_x) 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. 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. Experimental setup

Fig. 1 shows the schematic of engine which is single cylinder diesel engine with a displacement of 0.498 liters. The engine specifications are showed in Table 1. From the left side of schematic, intake system, engine and exhaust system were shown. Air was supplied from the intake system with naturally

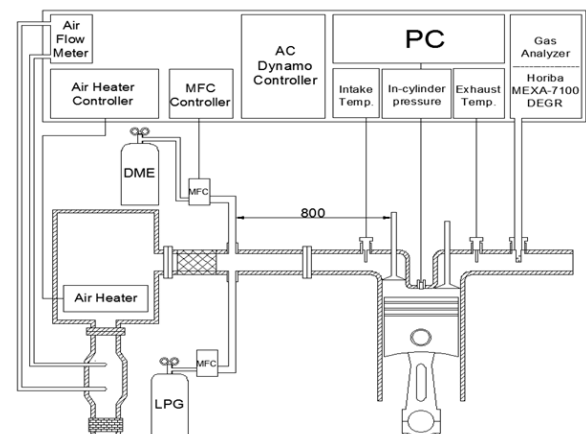


Fig. 1 Schematic of the engine facility.

Table. 1 Engine specification.

Displaced volume	498cc
Stroke	92mm
Bore	83mm
Connecting Rod	145.8mm
Compression ratio	14.5:1
Number of valves	2
Inlet Valve Close	-136° ATDC
Exhaust Valve Open	125.4° ATDC
Fueling system	Fully premixed

aspirated and metered by the air flow meter. Fuel was injected from the distance of 800mm of intake valve. The reason for the distance from intake valve was to maximize the pre-mixture of fuel and air. The temperatures for pre-mixture and exhaust gas were measured by the temperature sensors which were

AEC021

installed at intake valve and exhaust valve, respectively. In-cylinder pressure was measured by the pressure sensor which was located at the center of cylinder head.

2.1 Operational Conditions

In this study, DME and LPG was used as a fuel by injecting in the intake manifold to make the premixture. DME was main fuel. Dual fuel's mixing ratio was defined by the following equation and mixing ratios were shown in Table 2

$$\text{Mixing ratio of DME, } X_{\text{DME}} = \frac{\text{DME} \left(\frac{\text{g}}{\text{cycle}} \right)}{\text{DME} \left(\frac{\text{g}}{\text{cycle}} \right) + \text{LPG} \left(\frac{\text{g}}{\text{cycle}} \right)} \quad (1)$$

Table. 2 Mixing ratio definition

Mixing ratio of DME, X_{DME}	DME[%]	LPG[%]
1.0	100	0
0.9	90	10
0.8	80	20
0.7	70	30
0.6	60	40
0.5	50	50
0.4	40	60
0.3	30	70
0.2	20	80
0.1	10	90
0.0	0	100

2.2 Computational Approach

1) Chemical-kinetics modeling setup

The computational investigations have been conducted using the single-zone model of CHEMKIN [6] included in CHEMKIN-PRO [7-8]. 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 [9], using the geometry and specifications of the single-cylinder HCCI engine shown in Table I. The calculation starts from the intake valve close (IVC) of -136° aTDC to the exhaust valve open (EVO) of 125.4° aTDC. Chemical kinetic scheme was used from the mixing model which authors made in previous study and constructed from Curran's dimethyl ether (DME) and Kojima's n-Butane whose chemical kinetics mechanisms and thermodynamic parameters were used from Lawrence Livermore National Laboratory (LLNL) [10-11] and its properties showed in Table 3. DME fuel is considered a promising clean alternative fuel for ground transportation vehicles, and it can be substitute for conventional diesel fuel in a compression ignition diesel engine [12]. Autoignition process can be simplified by the extracting important reactions from detailed chemical kinetics mechanisms using

“contribution matrix to heat release” [13-14] as shown in Eq.2.

$$CHR_{j,n} = \frac{HR_{j,n}}{\sum_{j=1}^N \text{abs}(HR_{j,n})} \cdot 100\% \quad (2)$$

Here, CHR_{j,T_t} is the contribution ratio of j^{th} elementary reaction to heat release at a transient temperature T_t . HR_{j,T_t} is the heat release rate by the j^{th} elementary reaction at T_t . This study utilized the data for the value of contribution ratio to heat release of important elementary reactions above 3% at T_t .

2) Knock and misfire limits:

For this study, the ringing correlation developed by Eng [16] is used to quantify the knock level:

$$\text{Ringing Intensity} \approx \frac{1}{2\gamma} \cdot \left(\frac{0.05 \cdot \frac{dP}{dt, \max}}{P_{\max}} \right)^2 \cdot \sqrt{\gamma R T_{\max}} \quad (3)$$

Eq.(3) shows that the ringing intensity is proportional to the square of the absolute maximum pressure-rise rate (in kPa/ms). ($P_{\max}$ should be given as kPa, whereby Eq.(1) gives the ringing intensity in kW/m². The speed of sound comes in through the square root expression, and should be in m/s.) The use of a time based pressure-rise for computing ringing/knock is justified by the fact that the acoustic time scales are independent of engine speed. 5MW/m² was chosen as the limit for allowable ringing.

Table. 3 Fuel properties

Items	DME	n-Butane	Diesel	Gasoline
Molecular Formula	CH ₃ OCH ₃	C ₄ H ₁₀	n/a	n/a
Low Heat Value [MJ/kg]	28.8	45.8	42.7	43.2
Cetane Number	55-60	<10	40-55	13-17
LTHR/Total HR*100[%]	10~30	0~5	n/a	n/a
HTHR/Total HR*100[%]	70~90	95~100	n/a	n/a

3. Results and discussion

1) Effects of mixing ratio on combustion phasing and emission characteristics:

Fig. 2 shows the combustion characteristics for the change of mixing ratio of DME and LPG at same input calorific value. In-cylinder pressure was increased till mixing ratio of 0.7 and decreased when mixing ratio was less than 0.6. The peak pressure was abruptly reduced as 4.19MPa from $X_{\text{DME}}=0.5$ and the amount of heat release was also decreased. From less than 0.4 of mixing ratio, the in-cylinder temperature was lower than 1100K.

AEC021

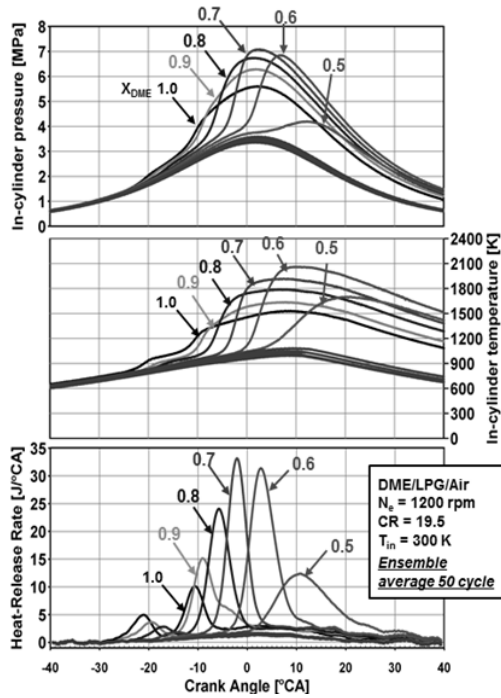


Fig. 2 Effect of mixing ratio on in cylinder pressure, temperature and heat release.

Fig. 3 shows the IMEP and thermal efficiency for the various mixing ratio. COV of IMEP took its peak at $X_{DME} = 0.5$ as 42% while its normal value should be within 8% [18-19]. As mentioned before, the ratios lower than 0.5 resulted the misfire operation. Therefore, IMEP was the highest at 0.6 for considering above conditions, where IMEP and thermal efficiency were increased by 250kPa and 28.2%, respectively, compared to $X_{DME} = 1.0$.

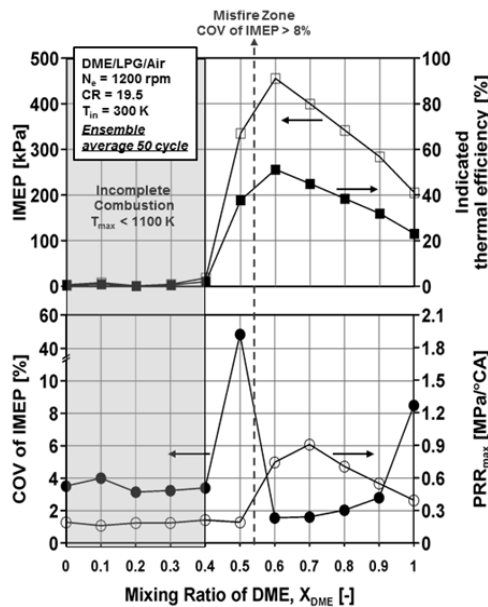


Fig. 3 IMEP, Indicated thermal efficiency, COV of IMEP and Maximum pressure rise rate for mixing ratio of DME

From the data-set for emissions in Fig. 4, the amount of THC and CO was decreased at the combustion zone where the in-cylinder temperature was higher than 1500K. NOx emissions were resulted very low since the in-cylinder temperature was lower than 2200K all the cases of combustion zone. Typically HC and CO generated when the in-cylinder temperature was lower than 1500K due to the no decomposition process from H₂O₂ to OH at lean and cold side of cylinder [20-21].

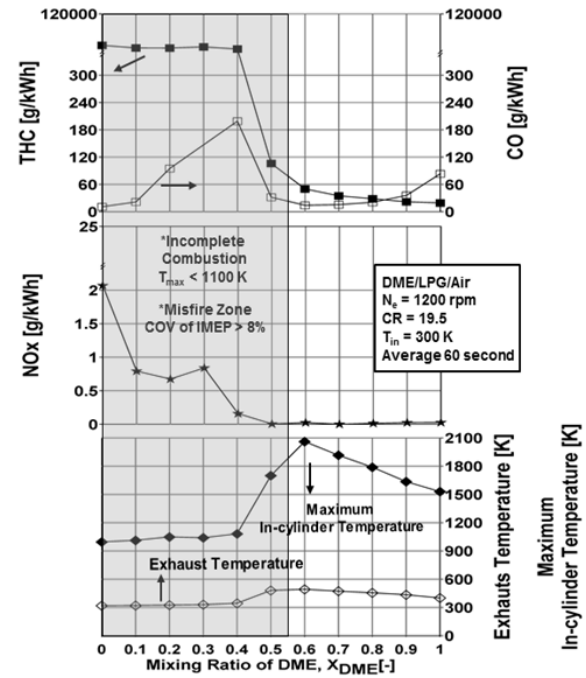


Fig. 4 THC, CO, NOx emissions, exhaust gas temperature and maximum in-cylinder temperature as a function of mixing ratio of DME

2) Effects of mixing ratio on controlled combustion phasing:

Controlling the combustion was conducted by holding the 50% burn point of heat release at bTDC 9°CA which is the case for input heat calorific value of 443J/cycle at $X_{DME} = 1.0$. Fixing CA₅₀ at same location reduces the variables for investigation and gives the potential to understand the correlation of parameters. For other mixing ratios, intake temperature was adjusted to obtain the identical CA₅₀. From the results, in-cylinder pressure was increased while LTHR was decreased as the increase of LPG amount as can be seen in Fig.5. Therefore, LTHR was abruptly reduced compared to the change of mixing ratio case and increases dramatically the HTHR. The IMEP and thermal efficiency took their peak at the mixing ratio of 0.8 and combustion duration was very short as 3.3 deg. LTHR was weakened and accelerates the HTHR, which might be further increase in-cylinder pressure and IMEP. At the mixing ratio of 0.7, combustion was occurred without LTHR.

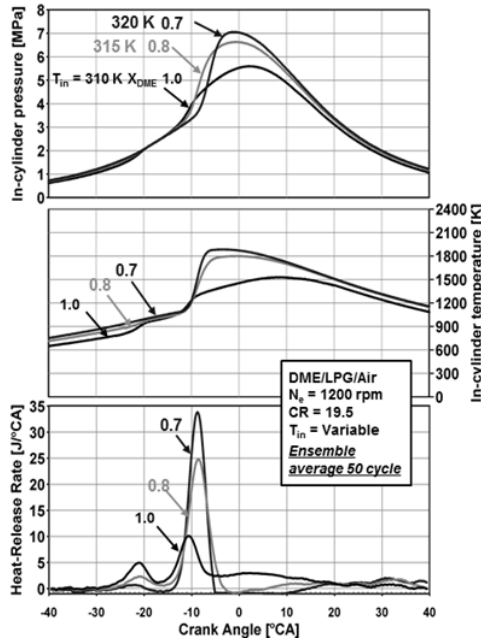


Fig. 5 Cylinder pressure traces, in-cylinder gas temperature traces, heat release rate and combustion duration for mixing ratio of DME at constant CA50 (-9 aTDC °CA).

3) Modeling results for the mixing ratio

The supplied fuel/ air equivalence ratio was 0.57 and intake caloric value was 770J/cycle throughout the change of mixing ratio to maintain the effect of fuel. Also, number of mole was fixed by the value of the base point which was selected for $X_{DME}=1.0$, 300K and 0.1MPa. Therefore, number of moles and intake calorific value were fixed constant by adjusting the intake pressure and temperature with the change of mixing ratio. Fig. 6 shows how intake pressure and temperature must be changed to obtain above mentioned baseline point and combustion duration and key combustion temperatures were shown. Therefore, in Fig. 7, mixing ratio 0.5 and 1.0 were compared to confirm the influences on autoignition and how it differs during the combustion process in view point of chemical kinetics.

Contribution matrix to heat release in which reactions were above the threshold as 3% was utilized and it gives the possibility to distinguish the important reactions participated in autoignition process of DME HCCI combustion. As can be seen in the Fig. 7, absolute heat release for overall dominant reactions and rates of those reactions in separate autoignition regimes for $X_{DME}=0.5$ and 1.0 were selected for the comparison. Among the fuel- series reactions, primary O₂ addition by 287 reaction and secondary O₂ addition by 295 reaction are dominant in cool flame. The equilibrium of these reactions shift toward the reactants side and the addition of O₂ to the alkyl radical is almost completely extinguished with the higher temperatures [26]. The temperature range for cool flame surrounded between 770K and 880K for $X_{DME}=1.0$ while it was started at 780K and transmitted at 860K to NTC range for 0.5.

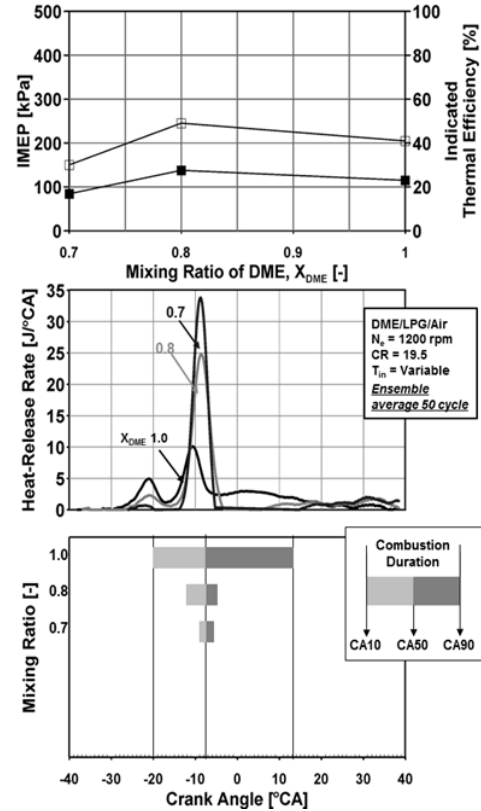


Fig. 6 Indicated thermal efficiency, Heat release rate, CA10, CA50, CA90 and Combustion duration for mixing ratio of DME at constant CA50(-9 aTDC °CA).

It was thought that the existence of n-Butane shortens the temperature range of cool flame. In case of NTC, it was terminated at 980K and 924K for the cases, respectively. Reactions went as similar trend to absolute HRR within these regions. Absolute HRR of primary O₂ addition reaction (287) was higher at $X_{DME}=1.0$ than that of 0.5 case. Around 860K for 0.5, decomposition reaction (294) was crossed with secondary O₂ addition reaction (295) and went upward since its forward reaction rate was increased, which was taken place around 870K for $X_{DME}=1.0$.

The role of TIP reactions is to increase the temperature to initiate the TI. After the fuel series reactions, H₂O₂ loop reactions were the main contributor to TI range in TIP range, which plays an important role in the thermal ignition by supplying heat rather than radicals. During the NTC range, almost reaction rates and heat release decreased but the only reaction was increased without falling down along with the increase of in-cylinder temperature which was H₂O₂ decomposition reaction (51) to generate OH. TIP begins around 980K and 925K after NTC in both cases. At $X_{DME}=0.5$, NTC was terminated at lower temperature and TIP was started and went through lower reaction rates, in which forward reaction rates were decreased as the increase of in-cylinder temperature. This is the reason of slowed down of autoignition with lower heat release and longer burn duration at TIP range. It can be also confirmed in combustion duration in Fig.2, where TIP was lengthened evidently at $X_{DME}=0.5$. In TI range,

AEC021

although there are a number of reactions contributed as plotted in the absolute heat release graph on top of figure, hydrogen-oxygen system reaction was initiated by the decomposition of H₂O₂ and the increase of OH, in which the competition of branching chain reaction (8) and HO₂ recombination reaction (26) are dominant along with temperature. As the temperature increase after TIP, reaction (51) of H₂O₂ loop was also contributor to take place of thermal ignition among the other reactions, of which reaction rates are higher than other reactions of loop. Reverse reaction rates of $X_{DME}=0.5$ had higher than that of $X_{DME}=1.0$ case

while it was inverse at forward reaction rate. This higher reverse reaction rate of H₂O₂ loop reactions at $X_{DME}=0.5$ case might be responsible for evidently longer TIP duration. At $X_{DME}=0.5$, combustion temperature was lower and duration of TI was longer even CA50 was identical with $X_{DME}=1.0$. At forward reaction rate of $X_{DME}=0.5$, the competition of reaction (8) and (26) was not strong and it terminates at lower temperature. It was thought the reason of increased duration of TI along with crank angle.

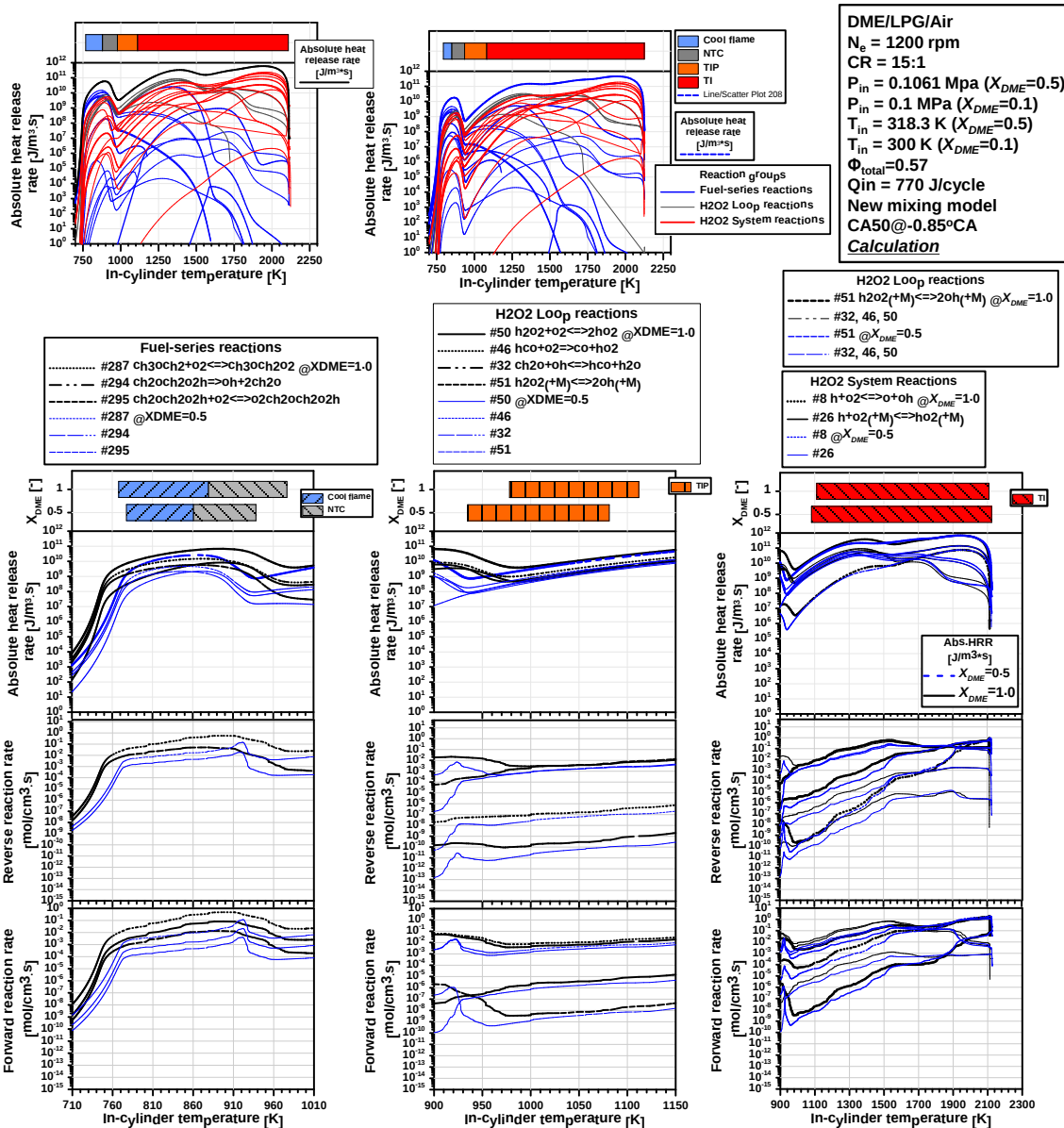


Fig. 7 Absolute HRR and reaction rates for dominant reactions in autoignition of DME/n-Butane HCCI combustion in case of $X_{DME}=0.5$ and 1.0.

4. Conclusion

In this work we attempted to increase the engine output by mixing of DME and n-Butane. Based on the experimental results, numerical work was conducted to understand the autoignition process in view point of chemical kinetics. Followings are concluded:

1) IMEP was increased slightly when X_{DME} was changed from 1.0 to 0.6 and took the peak value (455kPa) at mixing ratio of 0.6.

2) Thermal efficiency was similar trend with IMEP and had the minimum value at 0.6 as 51.2%.

3) The minimum values for THC and CO belonged to the mixing ratio of DME at 1.0 and 0.6 respectively. THC and CO were simultaneously reduced when X_{DME} was 0.8. NO_x almost does not existed.

4) DME and n-Butane mixture weakens the LTO reactions and decreases the temperature of HTO. However, reaction paths of the HTO were identical during the temperature from 1000 to 2100K.

5. References

- [1] Zhao, F., Asmus, T. N., Assanis, D. N., Dec, J. E. et al. Homogeneous Charge Compression Ignition (HCCI) Engines: Key Research and Development Issues, *SAE International*, Warrendale, PA, ISBN: 978-0-7680-1123-4, 2003, doi:10.4271/PT-94.
- [2] Yao, M., Zheng, Z., and Haifeng, L. Progress And Recent Trends In Homogeneous Charge Compression Ignition (HCCI) Engines, *Progress in Energy and Combustion Science*, 35(5):398-437, 2009, doi:10.1016/j.peccs.2009.05.001.
- [3] Eng, J. A. Characterization of Pressure Waves in HCCI Combustion, *SAE Technical Paper*, 2002-01-2859, 2002, doi:10.4271/2002-01-2859.
- [4] Cairns, A. and Blaxill, H. The Effects of Combined Internal and External Exhaust Gas Recirculation on Gasoline Controlled Auto-Ignition, *SAE Technical Paper* 2005-01-0133, 2005, doi:10.4271/2006-32-0042.
- [5] Zhao, H., Peng, Z., Williams, J., and Ladommatos, N. Understanding the Effects of Recycled Burnt Gases on the Controlled Autoignition (CAI) Combustion in Four-Stroke Gasoline Engines, *SAE Technical Paper* 2001-01-3607, 2001, doi:10.4271/2001-01-3607.
- [6] Kee, R. J., Rupley, F. M., Miller, J. A., Coltrin, M.E., et al., *CHEMKIN Release 4.1.1*, Reaction Design, San Diego, CA, 2007.
- [7] Kee, R. J., Rupley, F. M., and Miller, J. A. Chemkin-III: A fortran chemical kinetics package for the analysis of gas- phase chemical and plasma kinetics, *Sandia National Laboratories Report* No.SAND96-8216.
- [8] CHEMKIN-PRO, Release 15112, *Reaction Design, Inc.*, San Diego, CA, 2011.
- [9] Heywood, J. B. Internal Combustion Engine Fundamentals, *McGraw-Hill Book Company*, New York, USA (1998).
- [10] Fischer, S. L., Dryer, F. L., and Curran, H. J. The Reaction Kinetics of Dimethyl Ether. I: High-Temperature Pyrolysis and Oxidation in Flow Reactors, *Int. J. Chem. Kinet.* 32:713-740, 2000. *Lawrence Livermore National Laboratory*, Livermore, CA, UCRL-JC-239461.
- [11] Curran, H. J., Fischer, S. L., and Dryer, F. L. The Reaction Kinetics of Dimethyl Ether. II: Low-Temperature Pyrolysis and Oxidation in Flow Reactors, *Int. J. Chem. Kinet.* 32:741-759, 2000. *Lawrence Livermore National Laboratory*, Livermore, CA, UCRL-JC-239496.
- [12] Park, S. and Lee, C. Combustion performance and emission reduction characteristics of automotive DME engine system, *Progress in Energy and Combustion Science*, 39(1):147-168, 2013.
- [13] Kuwahara, K. and Ando, H. Role of Heat Accumulation by Reaction Loop Initiated by H₂O₂ Decomposition for Thermal Ignition, *SAE Technical Paper* 2007-01-0908, 2007, doi:10.4271/2007-01-0908.
- [14] Ando, H., Sakai, Y., and Kuwahara, K. Universal Rule of Hydrocarbon Oxidation, *SAE Technical Paper* 2009-01-0948, 2009, doi:10.4271/2009-01-0948.
- [15] Kuwahara, K., Tada, T., Furutani, M., Sakai, Y., et al. Chemical Kinetics Study on Two-Stage Main Heat Release in Ignition Process of Highly Diluted Mixtures, *SAE Technical Paper* 2013-01-1657, 2013, doi:10.4271/2001-01-0545.
- [16] Yamada, H., Sakanashi, H., Choi, N., and Tezaki, A. Simplified Oxygen Mechanism of DME Applicable for Compression Ignition, *SAE Technical Paper* 2003-01-1819, 2003, doi:10.4271/2003-01-1819.
- [17] Westbrook, C. K., Pitz, W. J., and Curran, H. J. Auto-ignition and chemical kinetic mechanisms of HCCI combustion, In: Zhao, H., editor. *HCCI and CAI engines for the automotive industry*. Boca Raton: Woodhead Publishing, p433-453, 2007.
- [18] Y. Nakamura, D.W. Jung and N. Iida. Closed-Loop combustion control of a HCCI engine with re-breathing EGR system, *SAE paper*, 2013-32-9069, 2013.
- [19] M. Sjöberg and J. E. Dec. Comparing enhanced natural thermal stratification against retarded combustion phasing for smoothing of HCCI heat-release rates, *SAE paper*, 2004-01-2994, 2004.
- [20] Y. Yamasaki and N. Iida. Numerical analysis of auto ignition and combustion of n-butane and air mixture in the homogeneous charge compression ignition engine by using elementary reactions, *SAE paper*, 2003-01-1090.
- [21] S. H. Kook, C. S. Bae, P. C. Miles, D. Choi and L. M. Pickett. The influence of charge dilution and injection timing on low-temperature diesel combustion and emissions, *SAE paper*, 2005-01-3837, 2005.