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Full Length Article

An investigation on the DME HCCI autoignition under EGR and boosted operation

Yanuandri Putrasari ^a, Narankhuu Jamsran ^a, Ocktaeck Lim ^{b,}*

^a Graduate School of Mechanical Engineering, University of Ulsan, Ulsan 44610, Republic of Korea **b School of Mechanical Engineering, University of Ulsan, Ulsan 44610, Republic of Korea**

highlights are the control of the control of

NTC temperature effects linearly on the rate of decomposition reaction for EGR.

• EGR reduces reaction rate of H_2O_2 loop during TIP in DME autoignition process.

Increased duration of TIP at boosting and EGR leads to reduce PRR.

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A numerical study was conducted to investigate the autoignition mechanism for controlling combustion phasing in a homogeneous charge compression ignition (HCCI) engine fueled with DME using zerodimensional commercial software in a detailed chemical-kinetics model and continued experimentally using single cylinder compression ignition engine. The exhaust gas recirculation (EGR) and boosting method where applied to control the combustion phenomena. The results indicate that EGR addition slows down the decomposition of hydrogen peroxide (H_2O_2) , which contributes to the amount of high temperature heat release by reducing the rate of hydroxyl radical (OH). Since too much EGR reduces the power and raises the carbon monoxide (CO), investigations focus on the autoignition characteristics of DME at boosting with EGR and their effects on variations of autoignition timings, combustion durations in two-stage combustion process in-detail using a contribution matrix to the heat release. It was found that longer duration of cool-flame with boosting due to increased oxygen concentration in the mixture, which finally enhanced the intermediate species reactivity but the duration of combustion dominantly depend on the EGR addition.

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1. Introduction

Advanced combustion strategies usually with low temperature combustion (LTC) process give the potential to meet the require-

E-mail address: otlim@ulsan.ac.kr (O. Lim).

ment for emissions legislation by avoiding to the use of after treatment system for cost reduction. LTC process is very interesting, due to its ability to achieve low particulate matter (PM) and nitrogen oxides (NOx) emissions to replace conventional diesel engine combustion. One of the several methods to obtain LTC in compression ignition (CI) engine is by using HCCI concept [\[1\].](#page--1-0) HCCI has been studied to find its appropriate technology with its own characteristics of the low emissions of the SI engine and the high efficiency of the CI engine [\[2\]](#page--1-0).

However, several technical issues related to HCCI engine concept must be fixed before mass production. High load operation limit from the excessive pressure rise rate (PRR) and ringing or knocking [\[3,4\]](#page--1-0) have been main problem since combustion strongly depends on chemical kinetics and thermodynamic characteristics of mixture. The purpose of using cooled EGR (external EGR) is to retard combustion by the means of controlling the heat release

Abbreviations: CR, Compression ratio; EGR, Exhaust gas recirculation; H_2O_2 , Hydroxyl peroxide radical; HC, Hydrocarbons; HCCI, Homogeneous charge compression ignition; HRR, Heat release rate; HTHR, High temperature heat release; IMEP, Indicated mean effective pressure; LTHR, Low temperature heat release; LTO, Low temperature oxidation; MPa, Mega Pascal; N₂, Nitrogen gas; NA, Naturally aspirated; N_e, Engine speed; NOx, Nitrogen oxides; NTC, Negative temperature coefficient; OH, Hydroxyl radical; P_{in}, Intake pressure; PM, Particulate matter; PRR, Pressure rise rite; SOI, Start of injection; TDC, Top dead center; THC, Total hydrocarbons; TI, Thermal ignition; T_{in} , Intake temperature; TIP, Thermal ignition preparation; ε , Compression ratio; φ , Equivalence ratio.

[⇑] Corresponding author at: School of Mechanical Engineering, University of Ulsan, 93, Dae-Hak Ro, Nam-Gu, Ulsan 44610, Republic of Korea.

over wide ranges of engine speed, lower the peak pressure, and further expanding the limits of high-load operation [\[5\]](#page--1-0). A combination of increase of specific heats capacity and reduction of oxygen (O_2) concentration associated with EGR addition results in suppression of autoignition and combustion-phasing retard, allowing high-load operation without knocking phenomena [\[6–9\].](#page--1-0) However, too much amount of EGR results the lower power output and increase the unburned carbon monoxide (CO) and hydrocarbon (HC) emissions since the constituents forming EGR such as $CO₂$ and $H₂O$ suffer the rapid burning rate. Therefore, one way to increase the load range is to increase the intake-pressure boost which intensifies the fuel autoignition reactivity.

Controlling the combustion phasing is particularly important under boosted conditions since the greater charge mass with boost increases the amount of pressure rise which is the main reason of knocking [\[10–14\]](#page--1-0). Also combustion phasing can influence on autoignition of HCCI process from any effect of engine operating conditions. Appropriate strategies of EGR and intake-pressure boost have the capability of extending the HCCI operation range to higher loads and further potential to be used in engines. The principal and control mechanism of EGR with boosting on HCCI autoignition should be able to explain in-detail for chemical kinetics across relatively wide ranges of operating parameters.

In this study, DME was used as a fuel, which is to be considered as an alternative fuel for land vehicles. In addition, it can replace the diesel fuel in a compression ignition diesel engine. The advantages of DME fuel are low autoignition temperature, high cetane number (above 55), low boiling point $(-25 \degree C)$, simple chemical structure and high oxygen content which result in soot-free engines combustion. In other hand, it can be generated from the various sources [\[15–17\].](#page--1-0) However, controlling the combustion phasing in DME HCCI engines with the combination of EGR and boosting should be understood in-depth. In this study, all data were obtained with CA50 5 \degree C A aTDC by adjusting initial temperature for avoiding the influence from combustion phasing retard, where it has been reported also that the highest power output could be obtained while maintaining the lower pressure rise rate (PRR) against ringing or knocking $[18]$. Therefore, it was chosen that the condition of combustion phasing at 5° C A aTDC for keeping as many operating parameters as possible constant.

Recently Kuwahara et al. [\[19\]](#page--1-0) developed the method called as ''Contribution matrix" to clarify detailed reaction paths of hydrocarbon fuels. Their method gives possibility to eliminate the unimportant reactions whose contribution ratios have less than threshold and to confirm the important reaction path from all reactions along with the histories of transient temperature in a reaction process. In their study, DME and n-heptane were chosen as a fuel in equivalent condition to the piston compression end at the compression ratio of 12:1 in a constant volume chamber. It was necessary to investigate in HCCI engine conditions since it uses very high compression ratio. Therefore, the objective of this research is to investigate experimentally and computationally the autoignition mechanism in DME HCCI combustion under EGR and boosting conditions.

2. Methodology

2.1. Experimental setup

DME HCCI combustion experiments were conducted on a single cylinder compression ignition engine which was modified from a four-cylinder diesel engine. Single cylinder (498 cm³) diesel engine with compression ratio of 19.5:1 was utilized for the current study. DME was injected directly into the cylinder with various injection timing for finding optimized injection location. DME was pressurized at 1.2 MPa by nitrogen. The reason is to keep the fuel in liquid phase for injecting precisely in short time during the engine cycles. DME fueling system consists of a tank, cooling system, check valves, visualization chamber (able to check fuel is in liquid state), high pressure pump (Haskel air driven pump), common rail and injector. Cooling system lowers the fuel temperature through the return line and keeps in liquid state until the accumulator. According to the problem from poor lubricity characteristics of DME, 1% mass of biodiesel was added to the DME fuel to increase the lubricity. Biodiesel contains oxygen atom which gives the potential to mix easily with DME. Flow rate of air was measured using a laminar flow meter (Meriam process tech.; Z50MC2-4) with the differential pressure transmitter (Yokogawa EJA110A) which is widely used to measure the air flow rate in the automotive field. In this study, coolant temperature and oil temperature were maintained constant to 80 ± 1 °C. Intake air temperature was kept constant at 25 ± 1 °C to supply into the engine. The engine is coupled to 57 kW AVL ELIN series 3 phase asynchrongenerator dynamometer (MCA-325M02) in [Fig. 1,](#page--1-0) which is a device for controlling the engine speed and measuring the torque (Torque) and the output (Power) in the whole range of speed and load that the engine is running. This study utilized $CO₂$ gas for EGR, which is pronounced as simulated EGR, instead of real EGR because $CO₂$ has the highest mole-specific heat capacity among other residual gases such as $H₂O$, N₂ and Ar [\[10\].](#page--1-0) EGR was supplied prior to the intake plenum as can be seen in the schematic of engine facility. EGR amount was controlled through the mass flow controller (Line Tech M3300V) for $CO₂$ gas. EGR rate was calculated by the Eq. (1) and Eq. (2);

$$
EGR[\%] = \frac{Q_{EGR}}{Q_{in}[noEGR] + Q_{EGR}} \times 100\%
$$
 (1)

$$
\mathbf{Q}_{\text{EGR}} = \left(\frac{\text{EGR}[\%] \times \mathbf{Q}_{in}[\text{noEGR}]}{100 - \text{EGR}[\%]}\right) \Big/ \left(1 + \frac{\text{EGR}[\%]}{100 - \text{EGR}[\%]}\right) \tag{2}
$$

where:

 $-$ EGR $[\%]$ = EGR rate

 $-Q_{EGR}$ = EGR flow rate

 $-$ Q_{in} [no EGR] = intake air flow rate without EGR.

2.2. Computational approach

2.2.1. Chemical-kinetics modeling setup

The computational investigations have been conducted using a single-zone model of CHEMKIN [\[20,21\]](#page--1-0) included in CHEMKIN-PRO [\[22\]](#page--1-0). The in-cylinder charge was treated as a mass of single lumped with thermodynamic properties and uniform composition in the single-zone model. The limitation in the single zone model calculations are in-cylinder temperature, pressure, composition assumed as homogeneous. Then, heat-transfer and blow-by effects were also not included. However, in this study the compression ratio was adjusted down to 14.5. This made the compression pressure match very well at TDC as can be seen as shown in [Fig. 2](#page--1-0), where the single zone model can be made to match the experimental pressure trace fairly during the compression and combustion event. This value is significantly lower than the experimental engine compression ratio of 19.5. The difference arises from heat-transfer and, to lesser degree, blow-by in the experimental case. The model is adiabatic and the lower compression ratio is therefore straightforward way to assure that the charge experiences the same pressure history as the experiment, without the complexity of applying heat-transfer to a single-zone computation. Based on the specifications and geometry of the single-cylinder HCCI engine and according to the standard slider-crank relationship, the compression/expansion was modeled and shown in [Table 1\[23\]](#page--1-0). The motored in-cylinder pressure validation method

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