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A 1-D Numerical Analysis on the Control of HCCI Combustion in a CI Engine Through Exhaust Gas Recirculation

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Keywords： HCCI, exhaust gas recirculation, combustion control, engine 1-D simulation.

ABSTRACT

In this study, we investigated the potential of combustion control of a diesel engine operating in homogeneous charge compression ignition (HCCI) mode through 1-D engine gas dynamic simulation (AVL BOOST). Effects of parameters including the content of residual gas, the ratio of external EGR, and its temperature on engine thermal efficiency were studied. The results showed that the engine efficiency increased with more residual gas at lean conditions. The temperature of recirculated exhaust gas is an important parameter for auto-ignition timing control. As the exhaust gas temperature becomes higher, combustion initiation occurs earlier, further results in the reduction of engine efficiency. The indicated efficiency of the engine operating in HCCI mode peaks at 43.19% with lambda of 3.53 without EGR. The simulation predicts that the efficiency can be improved to 44.07% by using leaner mixture and EGR.

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INTRODUCTION

Since its invention in 19th century, internal combustion engine (ICE) has been the major power source for transport systems, marine ships, agriculture machines, electric generators. Traditionally, ICEs are classified into two types: spark ignition (SI) engine, and compression ignition (CI) engine. SI engines use high octane number fuels like gasoline, alcohols, natural gas, liquid petroleum gas (LPG), and hydrogen. CI engines use high cetane number fuels such as diesel, biodiesel, dimethyl ether (DME). Efficiencies of CI engines are generally higher comparing to SI engines; however the NOx and particulate matters (PM) from this type of engine is very high. Expensive catalyst systems, such as lean NOx trap (LNT), selective catalytic reduction (SCR), diesel particulate filter (DPF), have to be installed to reduce these pollutants.

Homogeneous charge compression ignition (HCCI) has been considered to be a promising engine combustion technology that can avoid hazardous emissions without sacrificing efficiency. The concept of an HCCI engine is a combination of SI and CI engines. In an HCCI engine, charge mixture is premixed before being auto-ignited near top dead center (TDC) at the end of compression stroke. HCCI engine can work with both types of fuel. It can get high efficiency like CI engine and low NOx and PM like SI engine. The principle is also under many different names; for example, CAI, PCCI, PCI, ATAC, UNIBUS, PREDIC, NADI and MK (Zhao 2007).

Despite the advantages, there exist a lot of challenges such as operating range, engine vibration, and high CO and HC emissions, especially combustion control for HCCI engines. Due to the HCCI combustion onset by the in-cylinder temperature and mixture condition, chemical kinetics, not control directly by spark ignition time or injection timing like SI and CI engines. The performances of HCCI engine determined by CA50 position, the crank angle when 50% of fuel was burned. The thermal indicated thermal efficiency reached peak with CA50 in range 5 to 8 degree after TDC (Thanapiyawanit and Lu 2013). For this reason, control combustion timing is the first and the most important challenge of HCCI, there are several solutions have been proposed: changing compression ratio (CR), inlet air/mixture temperature, fuel system, EGR ratio, and compression efficiency.

With the same initial condition of inlet charge, the compression ratio strong effects on the in-cylinder temperature as well as auto-ignition timing. Hence, several studies investigated HCCI combustion characteristics on variable compression ratio (VCR) engines, and found that the combustion starts earlier with higher CRs (Olsson, *et al*. 2002, Haraldsson, *et al.* 2002). The compression efficiency, the ratio between dynamic CR to engine CR, also influences on the auto-ignition timing, with dynamic CR is the ratio of cylinder volume at IVC to volume at TDC. The inlet air/mixture temperature can evaluate the in-cylinder temperature to achieve HCCI combustion mode, for this reason, several researches on the influence of inlet temperature on HCCI combustion have been publish (Persson, et al. 2004, Maurya & Agarwal 2011). Dual-fuel system, injection strategies also is a potential solution to control the combustion phase in HCCI engine by mixture stratification or different octane number. By changing the amount injected two fuels and timing, the combustion phase can be controlled (Dec & Sjöberg 2004, Inagaki, *et al.* 2006).

Many research efforts have shown that EGR is one of the most promising approach for combustion control in an HCCI engine. Chen and Milovanovic (2002) used SENKIN to analyze the influence of burned gas by changing valve timing of a methane-fueled HCCI engine under stoichiometric condition. The compression ratio was 15, and the engine speed was 1800 rpm. The results showed that with a higher in-cylinder temperature, the ignition timing is advanced. When EGR ratio was less than 45%, mixture temperature was not enough for auto-ignition. The authors also considered the effect of the temperature of the recirculated exhaust gas (T_{EGR}) by fix EGR ratio at 50%. When T_{EGR} was increased from 750 K to 950 K, the combustion occurs earlier. Through 1D simulation software, Ricardo WAVE, the authors concluded that the variation of intake valve timing helped extend load range and reduce pumping work, the engine obtained higher efficiency when using variable valve timing (Mahrous *et al.* 2009).

Lu *et al.* (2005) studied the impact of operating conditions and EGR on HCCI combustion. In this study, the authors investigated the effect of EGR ratios, inlet air temperature, cooling water temperature, and engine speed on HCCI combustion characteristic. Mass flow rate of fuel is fixed at 18.88 mg/cycle, inlet air temperature is in the range between 28 and 32 ^{o}C. Authors also used the fuel with different octane number by changing the ratio of n-heptane and iso-octane. The results showed that increasing EGR ratios resulted in delayed start of combustion and longer combustion duration. Lu *et al.* (2006) also studied the impact of cooling water temperature on pressure and rate of heat release (ROHR) curves of an HCCI engine powered by primary reference fuel (PRF90) plus 3% di-tertiary butyl peroxide (DTBP). The results showed that the trend is similar.

Jang and Bae (2009) analyzed the impact of valve timing on efficiency of HCCI engine fueled with DME. Engine efficiency declined with lower valve lift due to earlier start of combustion. Whereas combustion efficient increased by the heat from residual gas trapped in cylinder, because valve opening duration is short and valve lift is small. Efficiency increased with advanced openings of intake and exhaust valves. At high load, engine had higher efficiency with higher valve lift and at lower load, the small valve lift is more suitable. Whereas, Milovanovic *et al.* (2004) used valve train system to control HCCI engine fueled with a high octane number fuel, RON95 gasoline. The results showed that valve timing have a large effect on gas exchange process, so it directly affected engine power, volumetric efficiency and load range. The residual gas will change the temperature of mixture at the beginning of compression stroke, which leads to the change of the auto-ignition timing. The influence of intake valve opening time and the mass flow rate of fuel on emission and combustion process in HCCI engine under dual-fuel model was also investigated with LPG and gasoline (Yeom *et al.* 2007). Peak pressure in a gasoline fueled HCCI engine is lower and combustion started later when intake valve opened late because of the low compression efficiency and volumetric efficiency. When intake valve opened early, indicated mean effective pressure (IMEP) was reduced due to early start of combustion and increased pumping work. However, engine power declined due to the incomplete combustion when the valve opened late. With a single cylinder engine fueled with acetylene, EGR technology was developed. Engine was equipped heating system to find the suitable temperature to get highest efficiency. The authors then adjusted EGR system (low and high temperature) to improving thermal efficiency and extend load range. By using a suitable EGR ratio, the range of engine load can be extended by 28%. Across the whole load range, combustion timing can be optimized resulting in improved engine thermal efficiency (Sudheesh and Mallikarjuna 2010).

The concept of using EGR to control combustion process in an HCCI engine was also studied by Nakano *et al.* (2000). The authors analyzed the potential of auto-ignition timing control while avoiding knock in an HCCI using EGR. Due to the dilution of burned gas, combustion started later, and pressure rise rate was reduced; therefore suppressing knocking. In experimental tests, the intake gas temperature increased with the application of EGR, and directly influenced the combustion timing. Hence, control both inlet air temperature and EGR ratios should be a feasible approach to get the optimized timing of ignition.

In this works, 1-D engine gas dynamic simulation was implemented to study the effect of EGR on HCCI engine performance. A model for a conventional CI engine was first constructed and validated. The model was then applied for HCCI mode. Results and discussion are presented in section 3. The last section showed the conclusions for this work.

RESEARCH METHODOLOGY

In the present study, the 1-D gas dynamic model of a CI engine (AVL-5402) was built on AVL BOOST software, as shown in Figure 1. The AVL-5402 engine is a single cylinder CI engine, using the common rail fuel system. It is equipped in the Internal Combustion Engines Laboratory of Hanoi University of Science and Technology (HUST) in Vietnam. The specifications of this engine are shown in Table 1.

Table 1. Engine specifications.

Model	AVL-5402
Type of engine	Single cylinder Compression Ignition
Bore	85 (mm)
Stroke	90 (mm)
Compression ratio	17.3:1
Displacement	510.7 (cm^3)
Intake valves	16 ^{o}CA bTDC-46 ^{o}CA aBDC
Exhaust valves	53.5 ^{o}CA bBDC-16.5 ^{o}CA aTDC

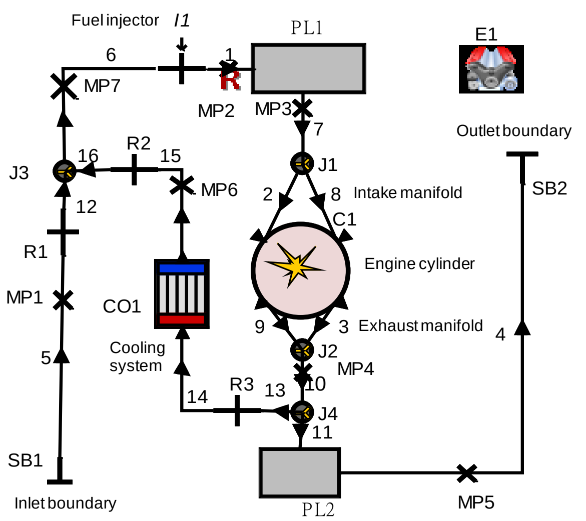

Fig. 1. AVL-5402 engine model on AVL BOOST.

In this model, air flow started from inlet boundary (SB1), passed the first restrictor (R1) and fuel injector (I1) to plenum (PL1). The gas (or mixture in HCCI mode) went to the junction (J1) and come to cylinder (C1) by two ports. The burned gas moved out through two exhaust ports, plenum 2 (PL2) and the exhaust pipes. When using EGR system, a portion of the exhaust gas enters intake manifold through junction 4 (J4), passed restrictor 3 (R3), cooling system (CO1), restrictor 4 (R4) and mixed with fresh air at junction 3 (J3). Seven measuring point (MP) were used in model to measure some parameters such as temperature, pressure, mass flow rate, and so on.

Under CI mode, the exhaust gas was not recirculated back to the intake manifold, i.e. the flow coefficients at two restrictors (R2 and R3 in the model) were set to 0. Moreover, no fuel was injected to the intake manifold from Injection 1 (I1 in the model). When operating in HCCI mode, the pressure of injected fuel was 60 MPa, and the injection timing was 20 ^{o}CA before TDC.

The combustion model utilized to predict the combustion characteristic of the DI engine is Mixing Controlled Combustion (MCC), developed by Chmela and Orthaber (1999). The model considers the effects of the premixed (PMC) and diffusion (MCC) controlled combustion processes according to:

$$\frac{dQ_{total}}{d\alpha} = \frac{dQ_{PMC}}{d\alpha} + \frac{dQ_{MCC}}{d\alpha} \qquad (1)$$

Compared to the experimental data at the same condition, the pressure profile from simulation was in good agreement with the experimental curve, as showed in Fig. 2. The comparison shows the validity of the model, which will be utilized to study the characteristics of the engine operating in HCCI mode.

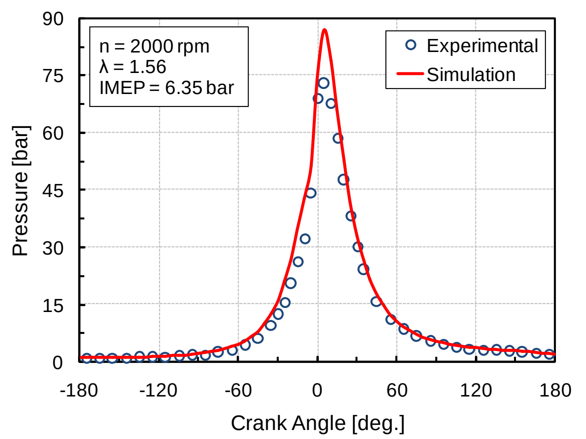

Fig. 2. Pressure curves from experiment and simulation data under CI mode.

The same model for CI engine was used for studying the characteristics of HCCI operation by changing the combustion model from MCC to HCCI and the fuel from diesel to n-heptane, C_7H_{16}, a diesel surrogate fuel. The fuel is injected from Injection 1 (I1 in Fig. 1). Table 2 shows the properties of this fuel. The HCCI model was based on a skeletal n-heptane mechanism with 26 species and 66 reactions developed by Gabriel (2006).

Table 2. N-heptane properties.

Name of fuel	n-heptane
Chemical formula	C_7H_{16}
Molar mass (g/mol)	100.16
Cetane number	56
Density (g/ml)	0.692
Low heating value (MJ/kg)	44.5
Latent heat (MJ/kg)	0.317
Air/Fuel ratio	15.132

Simulations were performed at four fuel mass flow rates (four original lambda values), different time of exhaust valve opening/closing (no change in cam profile, only adjusts the angle of exhaust camshaft as shown in Fig. 3), different EGR ratios, different T_{EGR} and at engine speed of 2000 rpm. The lambda is given by

$$\lambda = \frac{AF_{comb}}{AF_{stoi}} \tag{2}$$

where AF_{comb} is the Air/Fuel ratio of the mixture by mass,

AF_{stoi} is the stoichiometric Air/Fuel ratio by mass.

With different exhaust valve timing and EGR ratio, the lambda value is changed because the AF_{comb} is not constant. The "original lambda" terminology was used to represent the case without EGR and advanced exhaust valve timing. Based on the results, we can analyze the trends for auto-ignition timing, pressure rise rate, exhaust emissions, and especially thermal efficiency, η_{th}. These trends would be useful for tuning the engine in HCCI mode.

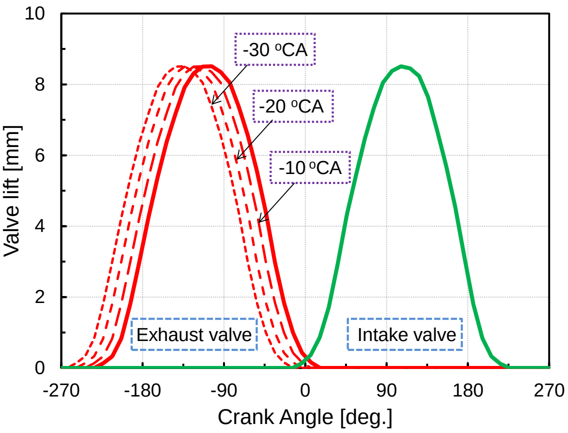

Fig. 3. The valve lift profiles for internal EGR studies.

RESUTLS AND DISCUSSION

Fig. 4 shows the pressure, temperature and ROHR profiles in HCCI mode at different lambda. The ignition timing is advanced and the pressure rise rate is higher, when the mixture is richer. Engine achieved highest efficiency with lambda of 3.53. With closer stoichiometric mixtures, the timing of auto-ignition is earlier because it has more radicals in mixture. The combustion velocity is also faster with these mixtures. The analysis shows that there are three stages of heat release, as can be seen in Fig. 4.

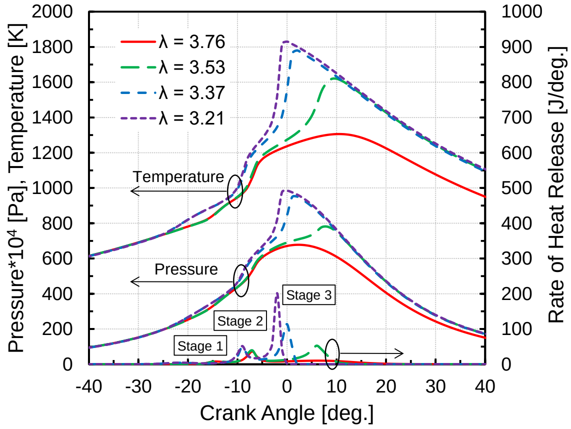

Fig. 4. The pressure, temperature and ROHR profiles at different value of lambda.

During Stage 1, which occurs at approximately -20 °CA, the fuel is first decomposed to C_7H_{15}, and then to $OC_7H_{13}O$, C_5H_{11}_1, nC_3H_7, C_3H_6, CH_2O, C_2H_4, and H_2O. The auto-ignition process is initiated. After that, nC_3H_7 is converted directly to C_2H_4, while $OC_7H_{13}O$ is converted to CH_2O, and then C_2H_4 and CH_2O are converted to CHO. The main source of heat release during this stage is from reaction of CH_2O to CHO, and CHO to CO through the following reactions:

$$CH_2O + OH \Rightarrow CHO + H_2O \tag{R1}$$
$$CH_2O + HO_2 \Rightarrow CHO + H_2O_2 \tag{R2}$$

and

$$CHO + O_2 \Rightarrow CO + HO_2 \tag{R3}$$
$$CHO + M \Rightarrow CO + H + M \tag{R4}$$

In Stage 2, nC_3H_7 is dissociated to C_2H_4 under the higher temperature. C_2H_4 further reacts with OH radical to generate C_2H_3, which is oxidized by O_2 through reaction R5:

$$C_2H_3 + O_2 \Rightarrow CH_2O + CHO \tag{R5}$$

CHO then reacts with H, OH, O_2 to produce CO.

The final heat release process (Stage 3) originates from the oxidation of CO to CO_2. The stage accounts for most of the heat release in the combustion process.

To study the effect of residual gas concentration on the combustion characteristics of HCCI engine, simulations at four different angles of exhaust camshaft were carried out, the in-cylinder pressure and ROHR profiles were presented in Fig. 5. When the exhaust valves open at 63.5, 73.5, and 83.5 degree of CA before BDC, the residual gas content was 1.77%, 3.39%, and 6.22%, respectively. The original fraction of residual gas is 1.26%. The residual gas content is the mass fraction of combustion products in the cylinder at the start of the high pressure phase (IVC). The residual gas content is given by

$$RG = \frac{m_{c,PC}}{m_{c,IVC}} \quad (3)$$

where $m_{c,PC}$ is mass of combustion products in the cylinder at IVC.

For the exhaust valve timing study, when λ = 3.53, the in-cylinder gas temperature at IVC is 352.11, 354.19, 363.07, and 380.91 K for original, advanced 10, 20, and 30 °CA of exhaust valve opening angle, respectively. Presence of residual gas, the ignition starts earlier because the initial temperature of the mixture is higher. However, with more residual gas, the combustion starts a little bit later due to the effect of heat capacity of burned products like CO_2, H_2O... The auto-ignition timing is 17.34, 28.29, 26.94, and 24.74 °CA BTDC with the opening time of exhaust valve is 53.5, 63.5, 73.5, and 83.5 °CA before BDC, respectively.

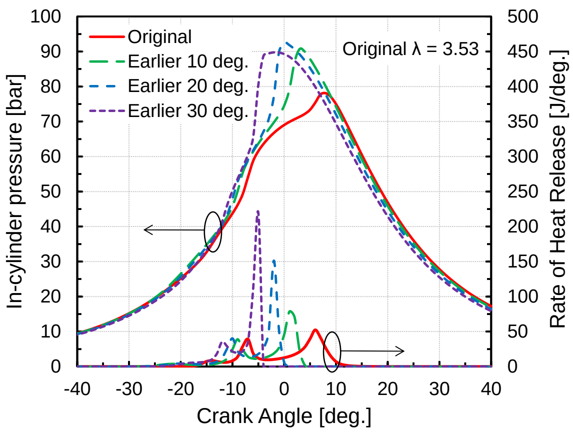

Fig. 5. Pressure and ROHR profiles at different timing of exhaust valve opening (original λ = 3.53).

The engine thermal efficiency, η_{th}, at four values of original lambda and four different opening angles of exhaust valve are shown in Fig. 6. Thermal efficiency reached peak with advanced opening time of exhaust valve (73.5 and 83.5 degree of CA before BDC) at extremely lean conditions (original lambda of 3.53 and 3.76) and vice versa. Due to the late combustion of leaner mixture, residual gas helps increase the mixture temperature, hence the auto-ignition phenomena occurs earlier.

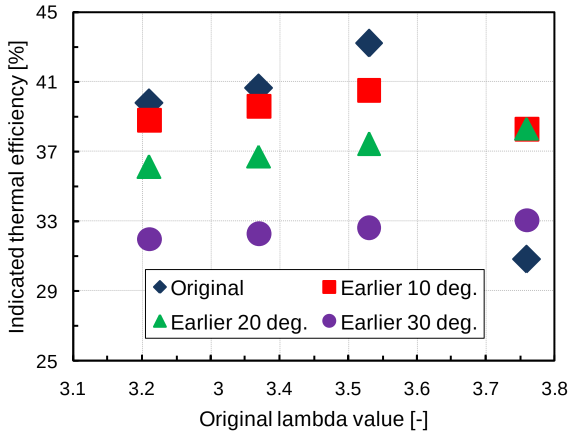

Fig. 6. Indicated thermal efficiency at different opening time of exhaust valve and original λ.

To study the effects of external EGR on engine characteristics, flow coefficients at R2 and R3 in Fig. 1 were adjusted to control EGR ratios, and temperature in cooler system (CO1 in model). The opening time of exhaust valve was fixed as the values shown in Table 1.

Fig. 7 presents pressure and ROHR curves at original lambda value of 3.53. Five EGR ratios were investigated and the EGR temperature (T_{EGR}) was fixed at 383K. The EGR ratio is defined by the following equation (based on the data from MP6 and MP7 in model).

$$\%EGR = \frac{\dot{m}_{EGR}}{\dot{m}_{EGR} + \dot{m}_{Air}} \times 100\% \quad (4)$$

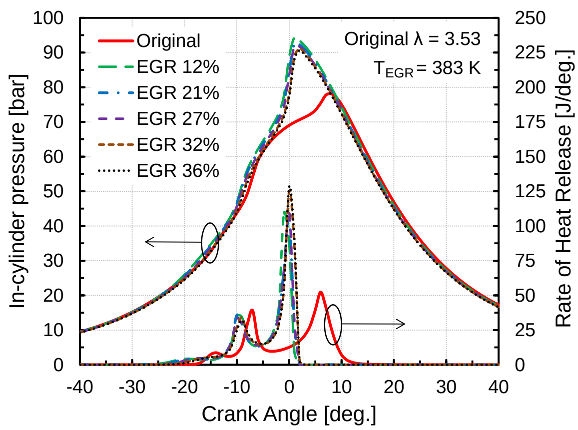

Fig. 7. Pressure and ROHR profiles at different EGR ratios and T_{EGR} = 383K (original λ = 3.53).

Because T_{EGR} is higher than fresh air temperature, the combustion starts earlier. The auto-ignition timing is 26.5, 25.83, 24.73, 23.2, and 22.74 °CA BTDC for EGR ratio of 12, 21, 27, 32, and 36%, respectively. Although the temperature of the inlet mixture is higher with more recycled burned gas, the high heat capacity of combustion products such as CO_2 and water vapor retards the auto-ignition timing. The overall effect results in a slightly later ignition as the EGR ratio exceeds 12%.

Fig. 8 shows the mass fraction of some species from 30ºCA before TDC to 30ºCA after TDC at original λ of 3.53, EGR 12% and T_{EGR} = 383K. Fig. 7 confirms that combustion starts 5ºCA in advance when 12% of the charge mixture is burned gas. The figure shows that CO and O_2 were reduced, whereas CO_2 and water vapor concentrations were increased, indicating more complete combustion.

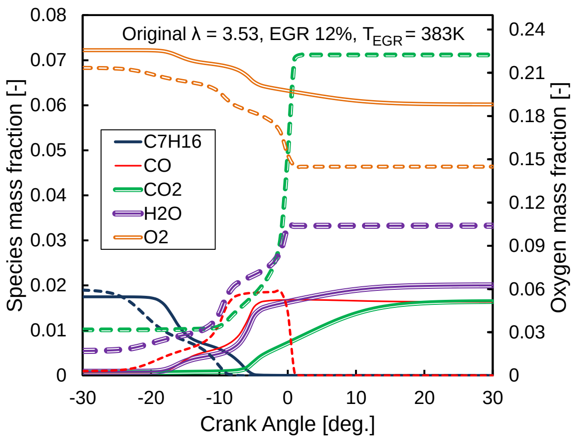

Fig. 8. Species mass fraction at original λ= 3.53 (solid line); EGR 12% and T_{EGR}= 383K (dash line).

Figures 9 to 12 show the engine thermal efficiencies at different EGR ratios and T_{EGR} and λ equal to 3.76, 3.53, 3.37 and 3.21. At extremely lean condition (original λ = 3.76) as demonstrated in Fig.9, using burned gas as an oxidant is an effective way to improve engine efficiency. However, at the original λ of 3.53, indicated thermal efficiency was not improved by EGR. With richer mixtures (λ = 3.37 and 3.21), using external EGR technology can help improve the engine thermal efficiency, especially with lower T_{EGR}, as shown in Fig. 11 and 12.

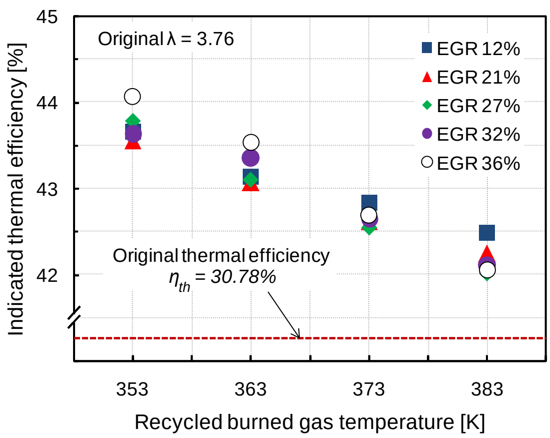

Fig. 9. Indicated thermal efficiency at different EGR ratios and T_{EGR} (original λ = 3.76).

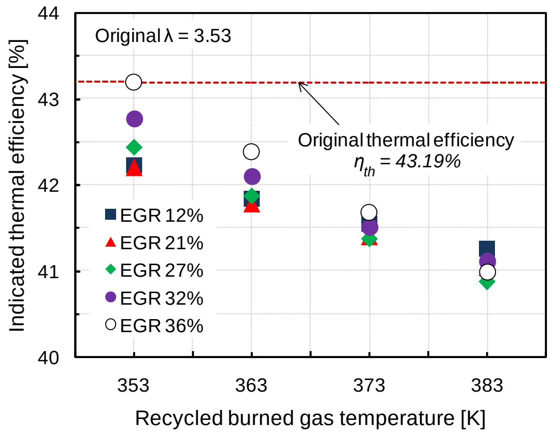

Fig. 10. Indicated thermal efficiency at different EGR ratios and T_{EGR} (original λ = 3.53).

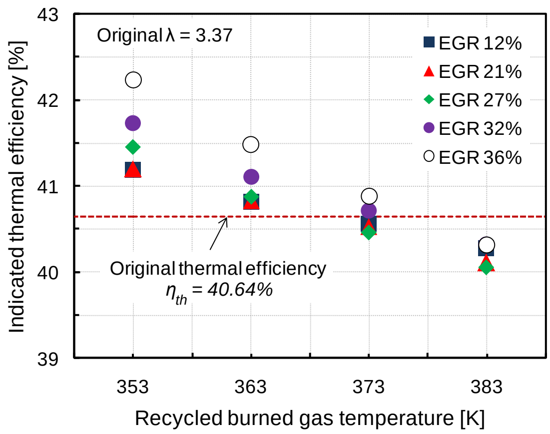

Fig. 11. Indicated thermal efficiency at different EGR ratios and T_{EGR} (original λ = 3.37).

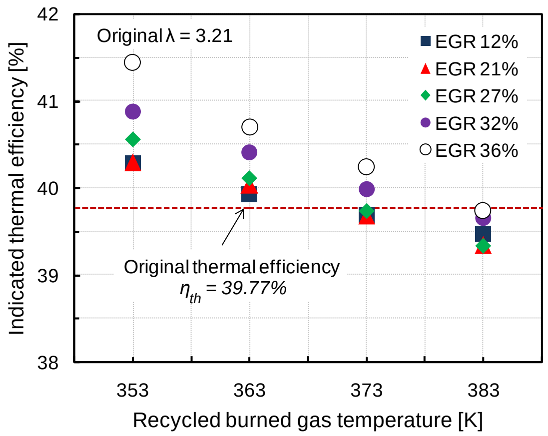

Fig. 12. Indicated thermal efficiency at different EGR ratios and T_{EGR} (original λ = 3.21).

Figures 9 to 12 also confirm that the engine thermal efficiency is higher with lower temperature of recyled burned gas. It can be explain by the fact that with lower temperature of mixtures, the ignition timing is later, therefore reducing the work for pumping. Additionally, volumetric efficiency of engine is also improved with the cooler flows.

CONCLUSIONS

One-dimensional engine gas dynamic simulations were performed as the first step of developing HCCI engine from a conventional diesel engine. The potential of combustion control by EGR technology were studied in this work. The simulation shows that the optimized lambda value is 3.53 for the engine operating in HCCI mode. The timing of auto-ignition is earlier with more residual gas due to the increase in mixture temperature. For a lean mixture of λ = 3.76, trapping burned gas in combustion chamber is an effective way to improve engine thermal efficiency.

When using the external EGR technology, the burned gas is cooled before being directed back to the intake. The temperature is still higher than the temperature of fresh air, so the start of combustion occurs earlier. Higher EGR ratio leads to higher charge mixture temperature, but the high thermal capacity of major recirculated burned gas species such as CO_2 and water vapor imposes adverse effect on ignition timing. Consequently, it is found that the ignition timing is the earliest when EGR ratio equals to 12%. External EGR is also a way to improve engine thermal efficiency when engine working in lean or rich conditions, comparing to the original λ of 3.53.

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NOMENCLATURE

1-D	one-dimension
ATAC	active thermo-atmosphere combustion
BDC	bottom dead center
CAI	controlled auto-ignition
CI	compression ignition
CO	carbon monoxide
DME	dimethyl ether
DPF	diesel particulate filter
DTBP	di-tertiary butyl peroxide
EGR	exhaust gas recirculation
HC	hydrocarbon
HCCI	homogeneous charge compression ignition
ICE	internal combustion engine
IMEP	indicated mean effective pressure
LNT	lean NOx trap
LPG	liquid petroleum gas
MCC	mixing controlled combustion
MK	modulated kinetics
NADI	narrow angle direct injection
NOx	nitrogen oxide
^{o}CA	degree of crank angle
PCCI	premixed charge compression ignition
PCI	premixed compression ignition
PM	particulate matter
PMC	remixed controlled combustion
PREDIC	premixed lean diesel combustion
PRF	primary reference fuel
RG	residual gas
ROHR	rate of heat release
RON	research octane number
SCR	selective catalytic reduction
SI	spark ignition
TDC	top dead center
UNIBUS	uniform bulky combustion system
VCR	variable compression ratio
λ	lambda – excess air to fuel ratio

以廢氣迴流控制壓燃引擎 HCCI 操作之一維數值分析

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摘 要

本研究之目的在於透過一維引擎氣動力模擬，探討不同比例的引擎廢氣迴流對於一 HCCI 引擎性能之影響。研究中探討了包括廢氣組成、迴流比例、殘餘氣體溫度等廢棄迴流參數對於燃燒起始時點與效率的影響。分析結果顯示引擎效率在貧油條件下會隨缸內已燃氣增加而提高。迴流廢氣之溫度為控制自點火時點之關鍵參數。較高溫度會使燃燒開始提前，造成效率降低。於 為 3.53 時，模擬所得最高效率為 43.19%，而當 為 3.76 時，迴流比為 36%及迴流氣溫度為 353 K 時，效率則提升至 44.07 %。