Reformer Gas Application in Combustion Onset Control of HCCI Engine

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Abstract

Homogenous charge compression ignition (HCCI) combustion is spontaneous multi-site combustion of a nominally premixed air/fuel mixture that exhibits high rate of pressure rise and short combustion duration. To avoid excessive pressure rise rate and knocking, HCCI engines are fueled with highly diluted mixture using a combination of excess air and/or EGR. HCCI combustion is attractive due to extremely low NOx emission output and high thermal efficiency but practical engines must overcome de-rating to a part-load power level and high HC and CO emissions. More importantly, HCCI engines lack a direct method of combustion timing control and this limits operating flexibility. One method of combustion timing control is to adjust mixture ignitability using a fuel blending agent with differing ignition properties than the base fuel. Reformer gas (RG) is a mixture of light gases dominated by hydrogen and carbon monoxide that can be produced from the base hydrocarbon fuels by several reforming techniques such as partial oxidation, autothermal or steam reforming. In a series of experimental studies, reformer gas was used to control combustion timing using a CFR engine and various base fuels: compressed natural gas (gas, high octane), iso-octane (liquid, high octane) and n-heptane (liquid, low octane). The effects of reformer gas on engine operating parameters and combustion characteristics were shown to differ for different base fuel. Keeping other influential parameters constant, increasing RG mass fraction in a natural gas mixture advanced combustion timing and shifted the operating range of the engine toward leaner mixtures. This enabled the natural gas-fueled HCCI engine to operate at leaner mixtures with decreased knock intensity and smoother combustion behavior. For iso-octane and n-heptane base fuels, combustion timing was retarded significantly as RG blend fraction increased. For the case of iso-octane the operating region did not change. However, for the n-heptane base fuel, the operating range was shifted toward richer mixtures, enabling higher indicated power and thermal efficiency. A chemical kinetic study of n-heptane / RG ignition showed that the influence of hydrogen was to suppress the first stage combustion and decrease the radical concentration after first stage combustion, thus delaying the main stage combustion, (despite faster major reaction rates during the main combustion period).

Keywords: Combustion, Reformer Gas, Hydrogen Enrichment, Combustion Control, HCCI Engine

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1. Introduction

Homogenous charge compression ignition (HCCI) is spontaneous multi-site flame-less combustion of a nominally homogenous highly diluted air/fuel mixture under controlled heat release condition. As HCCI combustion does not have flame propagation, high dilution of the cylinder charge with excess air and/or EGR is possible, leading to a low peak combustion temperature and very low NOx production. Also, HCCI permits the efficiency of Otto-cycle engines at low load to approach diesel levels by combining high compression ratio with rapid combustion, the avoidance of throttling and relatively low combustion heat losses. These attributes make HCCI combustion a key future technology for better and cleaner fuel utilization in an IC engine.

HCCI combustion first described in 1979 with a two stroke engine by Onishi et al [1] in a two-stroke engine and later by Najt and Foster [2] in a four-stroke engine. Subsequently, many studies have appeared and have been focused on addressing the HCCI combustion drawbacks of low power density, high HC and CO emissions, narrow operating range and lack of a direct method to initiate combustion. Spark ignition (SI) engines control combustion timing through spark timing and compression ignition (CI) engines do the same through fuel injection timing. The control of ignition timing is critical, achieving suitable combustion phasing over a range of conditions including speed, load, and temperature.

Among the HCCI combustion disadvantages, the most critical is the lack of a direct method to control combustion timing. HCCI combustion is a spontaneous auto-ignition which occurs at a time controlled by intake conditions (temperature and pressure), compression ratio, engine speed, air/fuel ratio, EGR fraction, fuel auto-ignition quality and degree of mixture homogeneity. While many adjustable engine parameters have some influence on ignition timing, none can directly control it. This leads to the classically narrow operating range for HCCI engines, where slight changes in influential parameters can shift the engine from severe knock to acceptable operation to complete misfire.

Several methods have been offered for HCCI combustion timing control. These can be classified as:

a) Methods that alter the end-of-compression temperature. As HCCI combustion is an auto-ignition, adjusting intake temperature or compression ratio can directly change combustion timing.

b) Methods that alter the combustion chemistry. As an example, mixing a high octane number fuel with a low octane fuel at various ratios can directly change combustion timing.

c) Methods that alter both thermal and chemical properties at the end-of-compression point. For example, changing the mixture air/fuel ratio and/or the EGR level can affect both ignition chemistry and post-compression temperature.

Most of these methods lead to further practical difficulties in engine control. For example, adjusting the intake temperature with a heater provides a fairly wide range of ignition timing control. However, the intake temperature adjustment rate is not fast enough to adjust for cycle-by-cycle variation or to stabilize combustion during engine load transients.

This paper is focused on HCCI combustion control in a dual fuel engine where two fuels with differing auto-ignition qualities are blended at varying ratio to control combustion timing. Control of fuel injection has the advantage of being sufficiently fast to change ignition timing on a cycle-by-cycle basis. Several previous studies have examined the possibility of the operation of a dual mode engine.

1.1 Dual fuel HCCI combustion engine

Various authors have shown that octane number is a poor predictor of HCCI combustion timing (see for example Aroonsrisopon (2002) [3]). However it has been shown that a binary mixture of fuels with known auto ignition qualities can be used to alter the combustion timing while not affecting other engine operating parameters. Olsson et al (2001) [4] used ethanol/n-heptane mixture to control HCCI combustion timing of a supercharged engine. Stanglmaier et al (2001) [5] operated a dual mode HCCI/SI engine with dual fuel concept (natural gas/naphta) in the HCCI mode with combustion timing control by fuel fraction adjustment. Dual fuel HCCI combustion was used with a series of different control techniques to control HCCI combustion timing on a cycle-by-cycle basis by Strandh et al (2004) [6].

The currently available fuel delivery systems and fast, precise control modules enable HCCI dual fuel engine operation. There is a practical barrier associated with carrying two fuels on board a vehicle or even delivering two fuels to a stationary engine. A solution to this problem is to supply a single base fuel and to use partial reforming of the base fuel to give a secondary, blending fuel with alternative combustion characteristics.

1.2 Reformer gas

Reformer gas (RG) is a mixture of light gases dominated by hydrogen, carbon monoxide and some quantity of inert gases such as carbon dioxide, nitrogen, and water vapor. Several

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previous studies used reformer gas or hydrogen to improve combustion stability (at extra lean or high EGR mixtures), decrease NOx, and improve cold start in conventional SI engines. RG can be produced from all hydrocarbons and/or oxygenate base fuels using various techniques such as partial oxidation, EGR reforming or steam reforming. Point-of-use or even onboard fuel reforming is a well-understood advanced technology where a great deal of progress has been made developing fuel processors for fuel cell applications. For details of reforming techniques see Jamal and Wyszynski (1994) [7], Dicks (1996) [8], Docter and Lamm (1999) [9], Pereira (1999, 2000) [10, 11], and Ogden (2001) [12]. It is worth noting that the performance of a fuel processor needed to provide RG as a fuel blending additive has considerably less critical specifications than one needed for fuel cell applications.

1.3 Reformer gas application in HCCI combustion

Application of RG in HCCI combustion engine has been studied using various base fuels. Shudo et al (2002, 2003, 2006) [13-15] have extensively studied the effects of methanol reformer gas on HCCI combustion of dimethyl ether (DME). The idea was to use methanol as the base fuel and convert it to RG and DME in a series of onboard fuel processers. In [13] effect of H2, CO and MRG (2H2 + CO) was studied on HCCI combustion of DME. It was found that adding any of H2, CO or methanol reformer gas (2H2 + CO) retarded the second stage of combustion, giving a less intense rate of pressure rise. The greatest effect belonged to H2 followed by MRG and CO. In [14] an onboard DME reformer was suggested.

Researchers at University of Birmingham have extensively studied reformer gas, EGR reformer gas, the effect of reformer gas on conventional combustion and the effect of reformer gas on natural gas HCCI combustion. In [16, 17] Peucheret et al (2004,2005) used exhaust gas reforming of methane to reduce the intake heating requirement of a natural gas HCCI combustion engine. They found that 10% H2 blending was sufficient for natural gas HCCI combustion and could be achieved through EGR reforming. Yap et al (2004, 2006) [18, 19] also reported that RG addition reduced intake heating requirement for natural gas HCCI combustion and was most beneficial at low loads. Several efforts by this group to expand the operating region of HCCI combustion by onboard reforming, trapping residual, and supercharging have been summarized in Xu et al (2007) [20].

Eng et al (2002) [21] studied the effect of partial oxidation reformer gas on two base fuels, (iso-octane and n-heptane), in an experimental and modeling study which explored the detailed chemical kinetic effects of H2 enrichment on the respective auto-ignition processes. The work showed strong effects of hydrogen on retarding and smoothing combustion with n-heptane when the engine used a well-mixed, external EGR supply. In contrast, the effects were minimal if the engine used exhaust re-breathing for EGR, presumably because the chemical kinetic effects were overtaken by fast auto-ignition at temperature inhomogeneities. With iso-octane fuelling, they found the engine would only run in HCCI mode with exhaust re-breathing and that RG replacement advanced and sharpened the HCCI combustion heat release.

At University of Alberta, the effects of simulated reformer gas on HCCI combustion have been studied extensively using a range of fuels, operating regions and initial conditions. Experimental results with natural gas HCCI combustion have been presented by Hosseini and Checkel (2006) [22], showing that RG advanced combustion timing and expanded the operating region toward leaner mixtures. At any constant λ and EGR, increasing RG fraction increased rate of pressure rise, increased NOx emission and decreased HC and CO emissions. HCCI combustion effects of RG replacement were also examined for a series of primary reference fuels (iso-octane / n-heptane blends), of varying octane level in Hosseini and Checkel (2007) [23, 24]. Effects of RG addition on n-heptane HCCI combustion was also studied by experimental analysis and modeling [25]. For low octane fuels, the dominant effects were found to be a reduction of low temperature heat release and retardation of main stage of combustion, resulting to a more optimized combustion timing. The effect was similar but much weaker using high octane fuels. Overall, it was found that RG was an effective combustion timing controller for a range of fuels.

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2. Experimental setup

A cooperative fuel research (CFR) engine was used for the purpose of this study. The CFR is a standard fuel research engine with bore × stroke of 3.25 × 4.50 inch and a displacement of 37.33 cubic inch, (0.62 litre). The engine intake system included an electrical air heater, a connection to an insulated EGR line with manually controlled butterfly valve and a set of port fuel injectors for gaseous or liquid fuels. The intake heater was controlled to keep intake mixture temperature, (including air, fuel, and EGR), was kept constant for each case. The constant mixture temperature is an important feature of this work as HCCI combustion is strongly affected by mixture temperature and the intent is to mimic a engine operating with preheated intake system where the only change from cycle to cycle is the ratio of RG fuel replacement. All tests were performed at steady state constant speed conditions. Fig. 1 and TABLE 1 show the details of experimental setup.

TABLE 1. Engine lab hardware description

Label	Description	Label	Description
1	Building pressurized air valve	7	Throttle
2	Air pressure regulator	8	Intake heater
3	High pressure safety valve	9	EGR valve
4	Low pressure safety valve	10,11	Fuel injectors
5	Intake Heater	12	Exhaust back pressure valve
6	Air drum	6	Intake air reservoir for mixing and pulsation damping

For the tests reported here, the engine intake was supercharged, (as described in [26]). The intake was pressurized to 50 kPa using building compressed air while an exhaust back pressure valve was adjusted to provide the proper EGR flow back to the pressurized intake. Supercharged HCCI operation is practically applied in real engines to raise the inherently low MEP of HCCI operation. In the experimental CFR engine, which has inherently high internal friction, supercharging provides enough indicated power to overcome the friction and study HCCI operation over an acceptable range.

Simulated RG was provided as a volumetric mixture H2 and CO, delivered from high pressure tanks. The RG mass fraction percent in total fuel was defined by: $RG_{mass,frac} = 100 \times \dot{m}_{RG} / (\dot{m}_{RG} + \dot{m}_{Fuel})$. λ was defined as relative air/fuel ratio considering fuel as both base fuel and RG. Any λ presented in this study is a total mixture strength considering base fuel and RG. Keeping λ constant and increasing RG mass fraction results in decreasing base fuel flow rate. Because the fuel may contain oxygen, the relative air/fuel ratio cannot be calculated in the normal manner, (Mueller 2005 [27]). Instead, the valence method was used. It calculates the equivalence ratio based on the valences of all atoms involved in the combustion equation. Using valence values of carbon (+4), hydrogen (+1), nitrogen (0) and oxygen (-2), the equivalence ratio was calculated as:

$$\frac{1}{\lambda} = \phi = \frac{\sum V^{+}}{\left|\sum V^{-}\right|}$$

where $\sum V^{+}$ and $\sum V^{-}$ are the summation of total positive valences and total negative valences of the intake mixture including both fuel and air respectively.

A Kistler 6043A water-cooled transducer was used to measure cylinder pressure with 0.1 CAD resolution. The throttle was kept wide open and cylinder pressure trace was referenced to intake plenum absolute pressure at intake valve closure. Pressure trace parameters were measured and calculated for 100 consecutive cycles and averaged. Other mean value parameters were measured by averaging over 50 consecutive cycles. The start of combustion was calculated by heat release using a zero-dimensional model considering air as the working fluid, (as described by Heywood (1988) [28]). Start of combustion was defined as 10% of total heat release and combustion duration was defined as the required crank rotation to complete the combustion from 10% of total heat release to 90% of heat release.

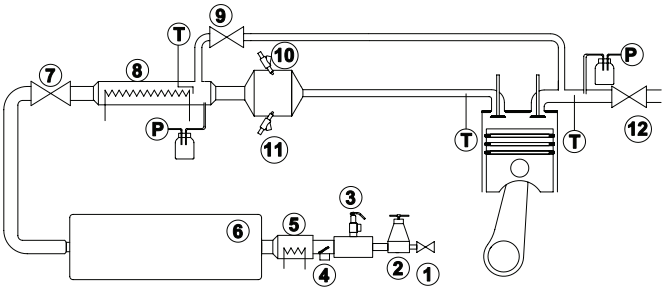

Fig.1. Schematic of the engine lab hardware, (described in table 1)

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3. Modeling description

A Matlab®-based, stand-alone chemical kinetic model was developed to investigate RG effects on reactions of natural gas and n-heptane in an HCCI engine. Model details can be found in Kongsereeparp and Checkel (2005, 2007) [29, 30]. The model, (named ChemComb), was capable of simulating complete cycles of an HCCI combustion engine using either single zone or multi-zone in-cylinder geometry, (SZM or MZM). The initial conditions of the model can be set by arbitrarily specifying pressure, temperature and equivalence ratio (φ) at intake valve closure, or by mass flow rates of intake mixture. The cited references show examples of ChemComb-SZM and ChemComb-MZM validation using pressure traces and engine operating parameters from the CFR engine. ChemComb-MZM uses novel approaches to set initial conditions, estimate inhomegeneity and optimize reaction rate coefficients, giving it a capability to predict experimental pressure traces with accurate ignition timing, combustion rate and subsequent engine performance. This predictive quality of ChemComb-MZM makes it a favorable choice for design purposes.

In this study ChemComb was used to examine the chemistry and thermodynamics of pre-combustion mixtures to illuminate the various mechanisms by which RG blending affected the combustion timing of natural gas HCCI. The ChemComb-SZM package was used for this since it is sufficiently accurate to model pre-combustion behavior and ignition timing. Due to it's single zone nature (having one zone and no inhomogeneity schemes for temperature, residuals, and φ, after combustion initiation, all of the mixture ignites simultaneously at a few computational steps. Consequently ChemComb-SZM over predicts cylinder maximum pressure, IMEP, and other engine parameters and under-predicts combustion duration. But as the purpose of modeling analysis was focused on the early stages of combustion, using ChemComb-SZM is accurate enough and computationally economic.

4. Effect of RG on HCCI combustion with natural gas base fuel

4.1 Natural Gas Base Fuel Operating Region

Experiments of natural gas HCCI combustion were performed at steady state conditions with N = 800 rpm, CR = 19.5, and $T_{intake,mix}$ = 140 oC. RG composition was chosen as 75% H2 / 25% CO and $RG_{mass,frac}$ was altered from 0% to about 40%. Fig. 2 shows the operating region of natural gas HCCI combustion with and without RG blending. Note that this is a typical HCCI combustion operating region, limited on the rich (higher power) side by knock and limited on the lean (lower power) side by partial burning and misfiring.

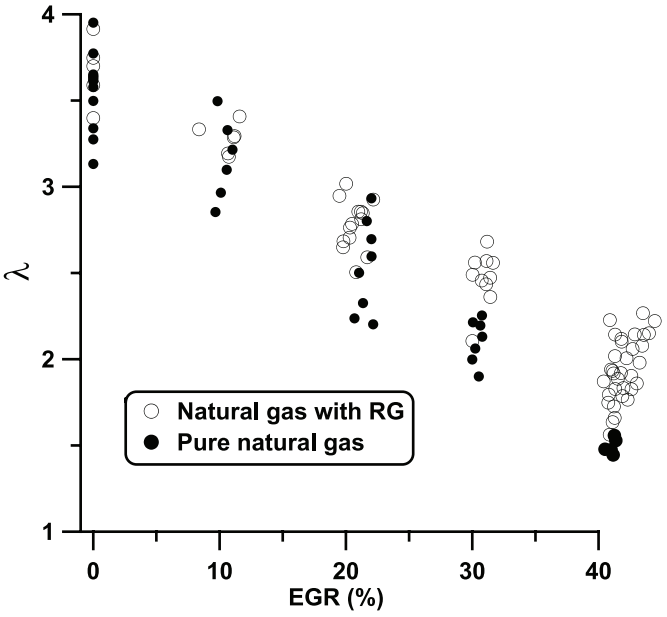

Fig.2. λ-EGR operating region of natural gas HCCI combustion with and without RG enrichment

Fig.2 shows that the HCCI operating region was expanded toward the lean side by using RG blending, especially at high EGR rates.

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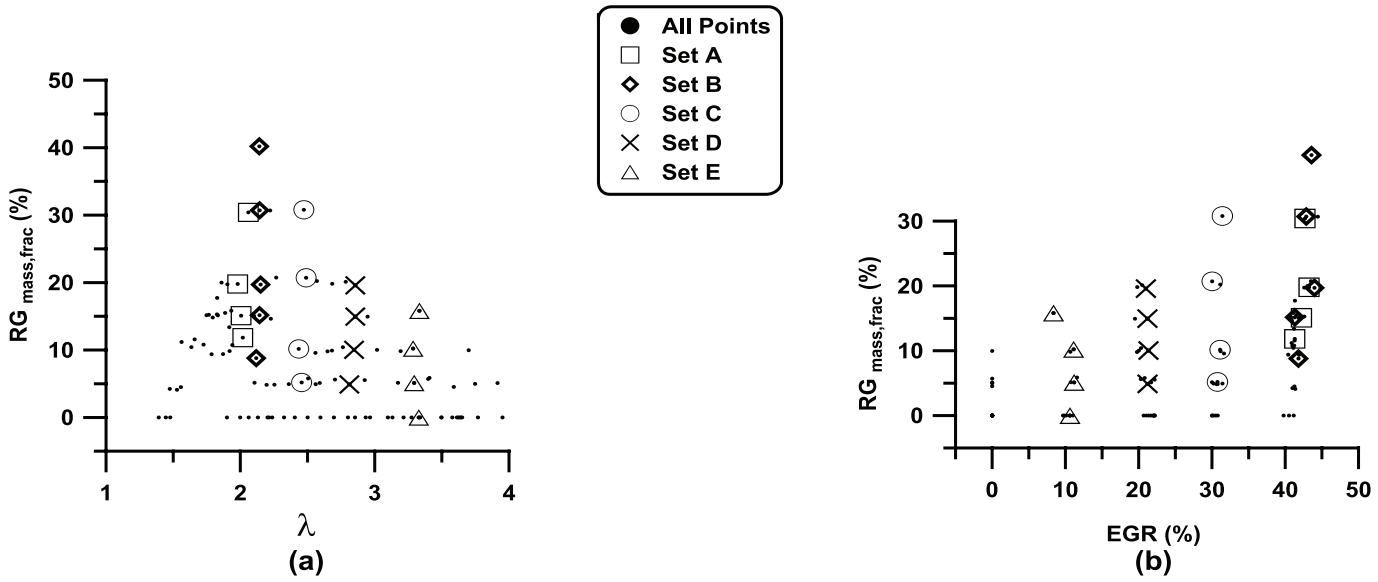

Fig.3. The operating region of natural gas HCCI combustion in the supercharged mode, (a) RG-λ operating points, (b) RG-EGR operating points, Symbols indicate constant λ group operating points that are defined in TABLE 2

The operating points shown in Fig. 2 used a range of $RG_{mass,frac.}$ Fig. 3 shows the relation of $RG_{mass,frac}$, mixture strength, λ, and EGR. Fig. 3-a and 3-b are two views of a three dimensional λ-EGR-$RG_{mass,frac}$ operating region. All possible RG enrichment fractions at high and low EGR and/or λ were tested. Increasing EGR made it possible to use higher $RG_{mass,frac}$ by pushing back the knock boundary at any constant λ. Increasing $RG_{mass,frac}$ at any constant Tintake,mix limited the operating region as indicated by the narrower λ range for high $RG_{mass,frac}$ in Fig. 3. For example, with 0% RG, HCCI operation was achieved between λ = 1.38 (knock boundary) and λ = 3.95 (misfire boundary). With 40% RG, the only possible fuel level was λ = 2.13. Fig. 3 also indicates five groups of approximate constant λ/EGR points for further analysis. These groups of data points are indicated by labels A to E as detailed in table 2.

TABLE 2. Selected groups of constant λ-EGR from natural gas HCCI combustion operating region indicated in Fig. 2. RG(%) varies for points in each set.

Label	EGR(%)	λ
A	42.5	2.02
B	42.7	2.13
C	30.8	2.46
D	21.1	2.46
E	10.3	3.31

4.2 Natural gas base fuel heat release characteristics

Fig. 4 shows the basic heat release parameters, start of combustion (SOC) and combustion duration (CD).

In general, increasing RG blending advanced SOC and reduced CD for the inherently high-octane natural gas fuel.

As an example, the pressure traces of data set B, (TABLE 2) are indicated in Fig. 5. At constant λ and EGR, increasing RG blending shifted the combustion pressure rise earlier in the cycle and increased peak cylinder pressure and maximum pressure rise rate. The pressure trace for 8% RG showed partial burning while that for 40% RG showed marginal knocking.

Fig. 6 shows the heat release curves for the set B of data points. Increasing RG blend fraction advanced timing of maximum rate of heat release (Fig. 6-a) and increased the rate of heat release.

The gross accumulative heat release curve, (an integration of net rate of heat release plus heat transfer to the cylinder walls), indicates shows the same behavior (Fig. 6-b).

4.3 Natural gas base fuel modeling results

The validation of the chemical kinetic and heat transfer model has been presented elsewhere (see Kongsereeparp and Checkel (2007) [31]). Fig. 7 shows the pre-combustion in-cylinder t emperature and specific heat ratio as a function of increasing RG blending ratio. As shown in Fig. 7-b, an increasing RG blend ratio raised the specific heat ratio of the mixture by replacing a complex fuel molecule with simple bi-atomic RG molecules (H_2 and CO). Hence, post-compression temperature was increased (Fig. 7-a) and ignition advanced as the RG blend fraction increased.

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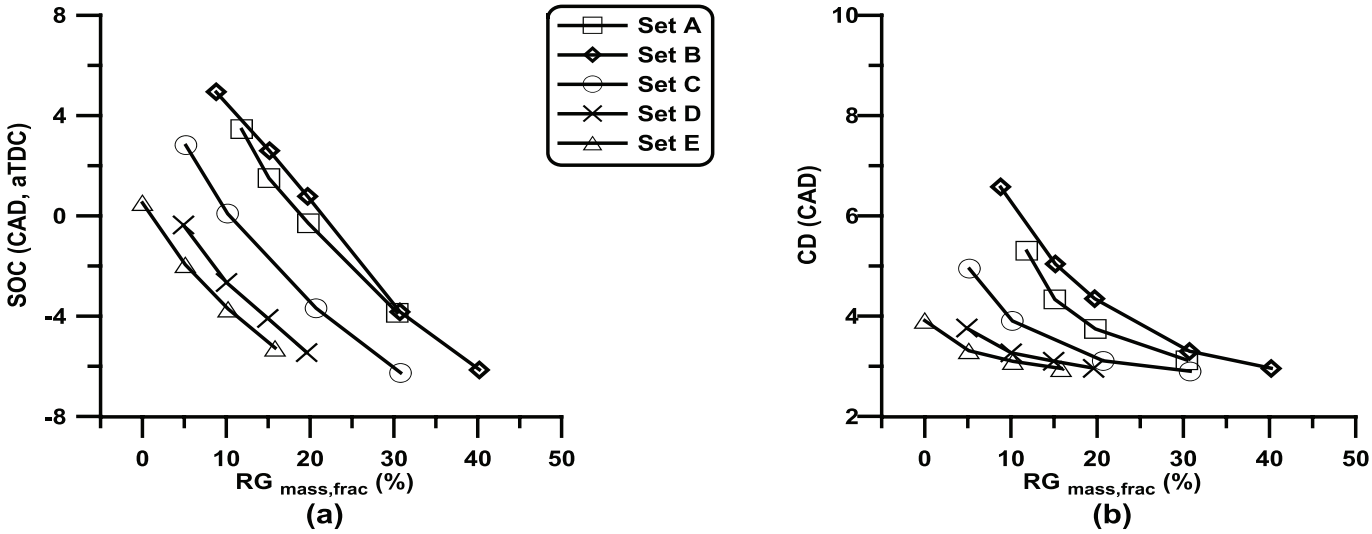

Fig. 4. Effect of RG on (a) start of combustion, and (b) combustion duration, HCCI combustion of natural gas for selected constant λ-EGR cases of TABLE 2

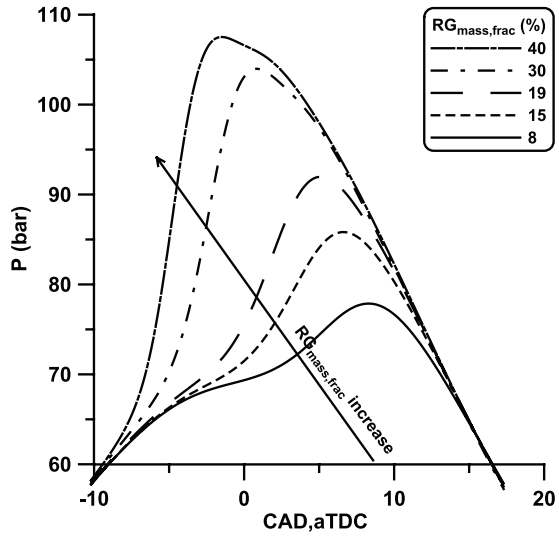

Fig. 5. Effect of RG on natural gas HCCI combustion pressure trace at constant λ and EGR, for group B of data indicated in TABLE 2

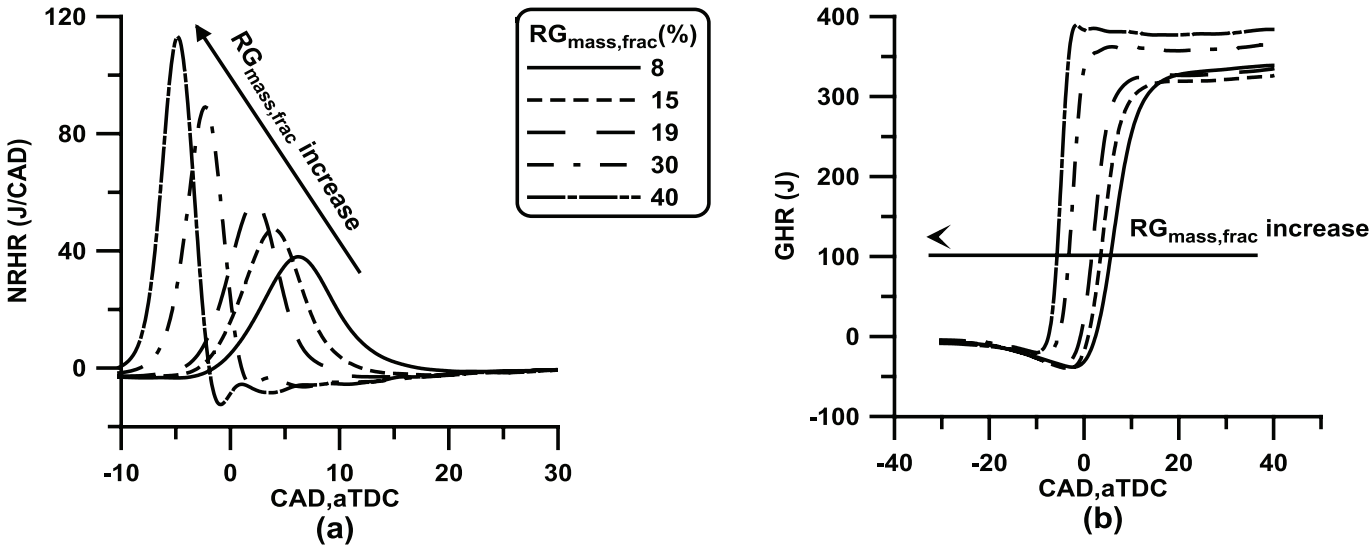

Fig. 6. Effect of RG on (a) net rate of heat release, and (b) gross accumulative heat release, natural gas HCCI combustion for group B of data in TABLE 2

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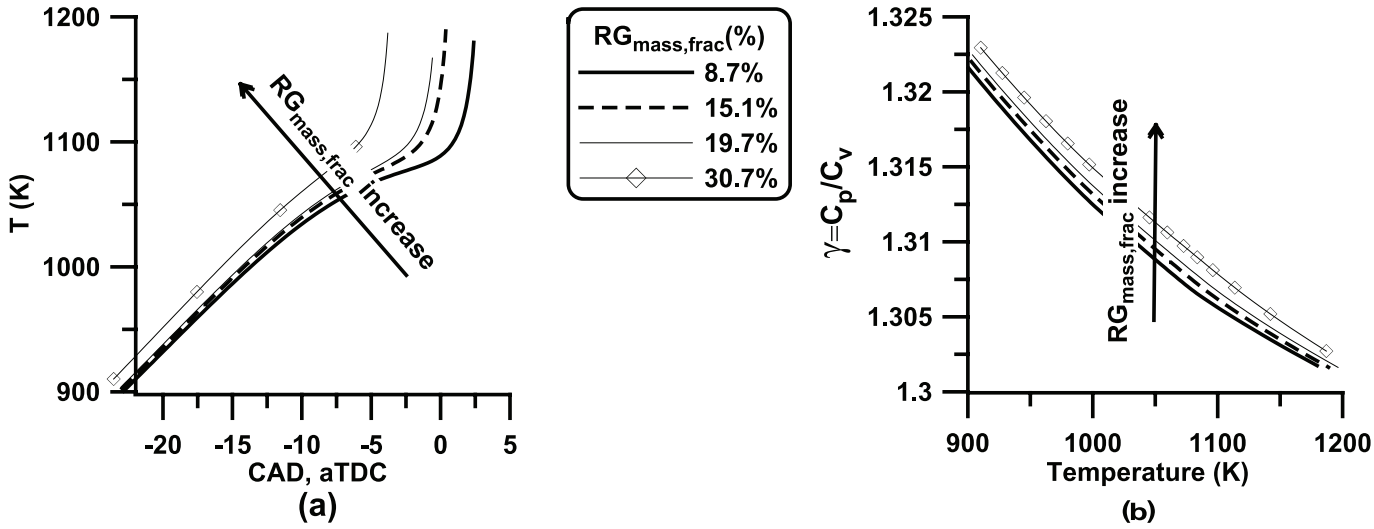

Fig. 7. Effect of RG on (a) in-cylinder temperature during compression and start of combustion, and (b) ratio of specific heats, HCCI combustion of natural gas simulated with ChemComb-SZM

4.4 Natural gas base fuel discussion

HCCI combustion of natural gas was difficult to achieve and exhibited a relatively narrow operating range in the CFR engine, even with supercharging. It was shown that increasing RG blending fraction, (while keeping all other influential parameters, λ, EGR, CR, speed, $T_{intake,mix}$, and intake pressure constant), advanced the combustion timing and shortened the combustion duration. Basically, the RG acted as a lower-octane blending agent and thus aided ignition for the very high-octane natural gas base fuel.

The combustion simulation showed that advancing combustion timing resulted from higher post-combustion temperature due to altered thermodynamic properties with RG blending. Replacing the base fuel, (methane), with RG, (H_2 + CO), raised the specific heat ratio of the compression mixture and thus significantly raised the post-compression temperature considerably. HCCI ignition is highly sensitive to temperature history, and natural gas chemical kinetics of combustion heavily relies on a single-stage combustion with no intermediate radical pool formation so post-compression temperature was the dominant factor.

All subsequent changes in engine operating parameters and combustion characteristics come from combustion timing alteration with RG. In [22] it was shown that at constant initial conditions, increasing RG blend fraction increased combustion intensity, in-cylinder maximum pressure and maximum pressure rise rate, while HC and CO emissions decreased, and NO_x emission was increased. This is in agreement with other studies that suggest H_2 addition to the intake mixture reduces intake heating requirements for natural gas HCCI combustion (e.g. [16, 17, 19]). In [19] Yap et al used an actual fuel reformer in a closed-loop system utilizing EGR reformer gas (REGR). Although their experimental setup was different from this study (intake temperature changed when adding RG), they reported that adding REGR advanced combustion timing and increased HC and CO emissions for HCCI combustion of natural gas.

5. Effect of RG on Iso-Octane HCCI combustion

5.1 Iso-Octane Base Fuel Operating Region

Iso-octane was used in these experiments to represent high octane fuels such as gasoline. Achieving iso-octane HCCI combustion is difficult due to high octane quality. Fig. 8 shows the achievable operating points for supercharged iso-octane HCCI, with and without RG enrichment.

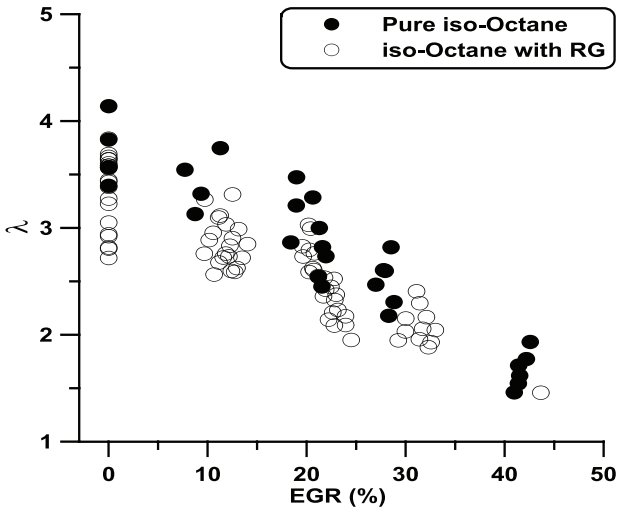

Fig. 8. λ-EGR operating region of iso-Octane HCCI combustion with and without RG enrichment

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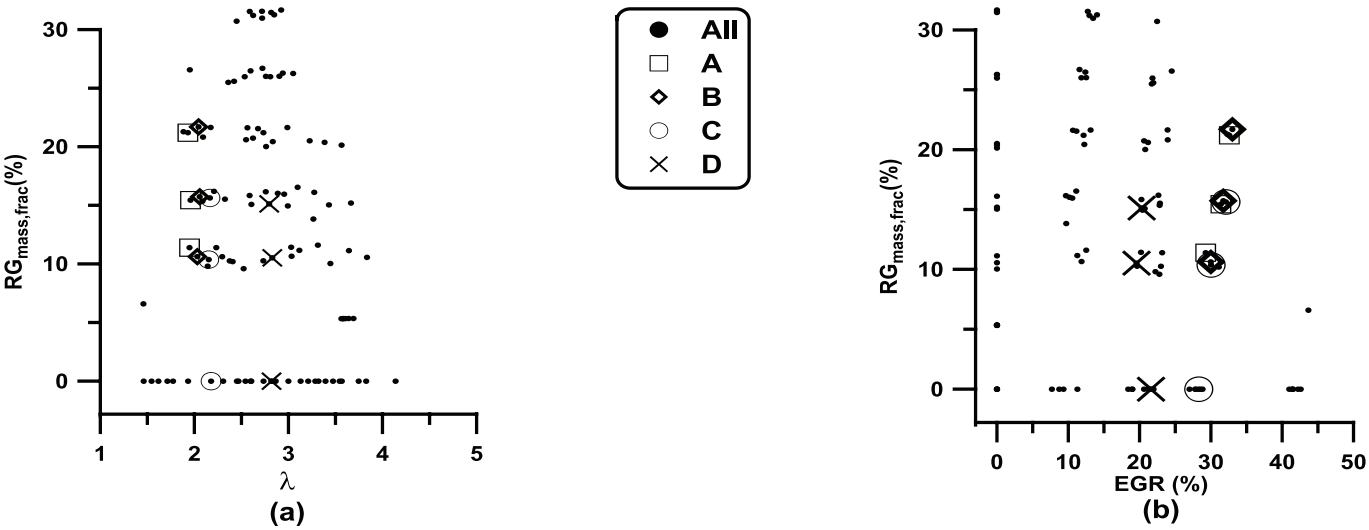

Fig. 9. (a) RG-λ and (b) RG-EGR operating regions for iso-Octane supercharged HCCI combustion with indication of constant λ-EGR groups of data defined in TABLE 3

At low EGR fractions, iso-octane base fuelling gave a significant HCCI operating range (between knock and misfire). For higher EGR fractions, the operating range narrowed. In general, RG blending shifted the allowable operating range toward the rich, (higher power) side by pushing back the knock boundary. This agrees with the results in previous studies with conventional engines, where some combination of RG or H_2 was used as a knock suppressor, (e.g. see Topinka et al (2004) [32]).

Fig. 9 shows the relation of RG blend fraction to λ and EGR. Fig. 9 is are two-dimensional views of a three dimensional RG-λ-EGR engine operating map.

Fig. 9 shows that with increasing RG blend fraction, the operating window narrowed on both the lean and rich sides. As shown in Fig. 9-b, increasing EGR fraction also limited the maximum applicable RG blend fraction. A series of data points with same values of λ and EGR are grouped in Fig. 9 and identified in Table 3.

TABLE 3. Selected groups of constant λ-EGR from iso-Octane HCCI combustion operating region indicated in

Label	EGR(%)	λ
A	31.0	1.94
B	31.5	2.04
C	30.1	2.16

5.2 Iso-Octane base fuel heat release characteristics

Fig. 10 shows the effect of RG blend fraction on the start of combustion and combustion duration for the selected λ-EGR cases identified in Fig. 9 and TABLE 3. Increasing RG blend fraction at constant λ and EGR postponed the combustion timing (Fig. 10-a), prolonged the combustion duration (Fig. 10-b) and increased combustion instability. The error bars on both SOC and CD plots are indication of cyclic variations calculated over 100 consecutive collected cycles and the larger error bars correspond to greater cyclic variation.

Fig. 11 shows the median pressure traces of the group C cases, (EGR = 30%, λ = 2.16), indicated in Fig. 9 and TABLE 3. At constant λ and EGR, increasing RG blend fraction retarded the cylinder pressure trace, decreased cylinder maximum pressure and reduced maximum pressure rise rate.

Fig. 12 shows the effect of RG on net rate of heat release and gross accumulative heat release for HCCI combustion of iso-octane. Increasing RG blend fraction decreased the maximum heat release rate and retarded the gross accumulative heat release.

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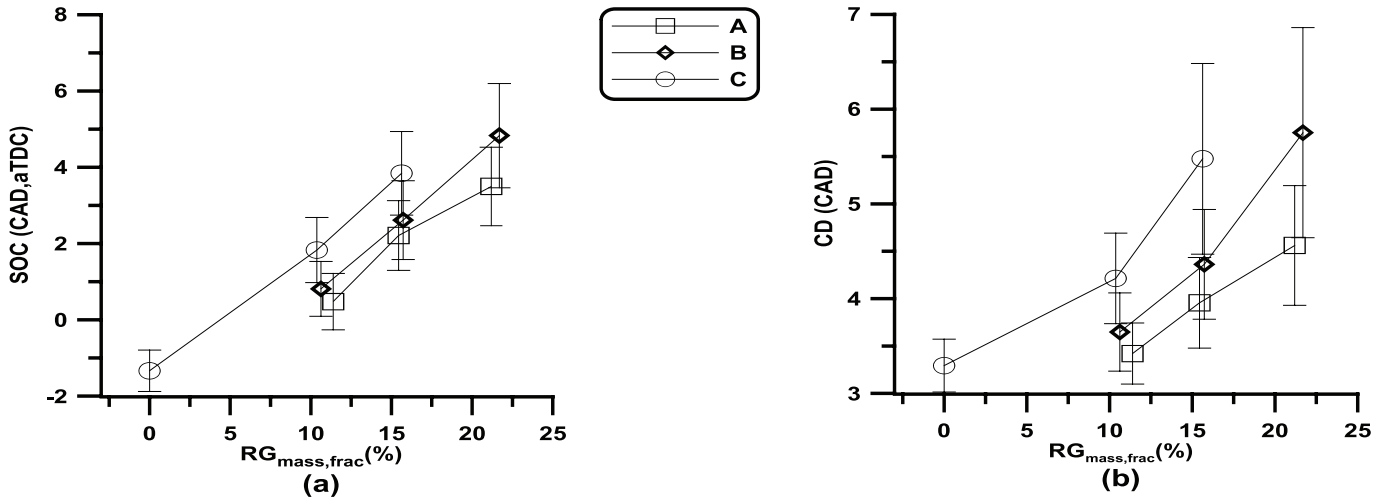

Fig. 10. Effect of RG on (a) start of combustion, and (b) combustion duration, HCCI combustion of iso-octane for selected constant λ-EGR cases of TABLE 3

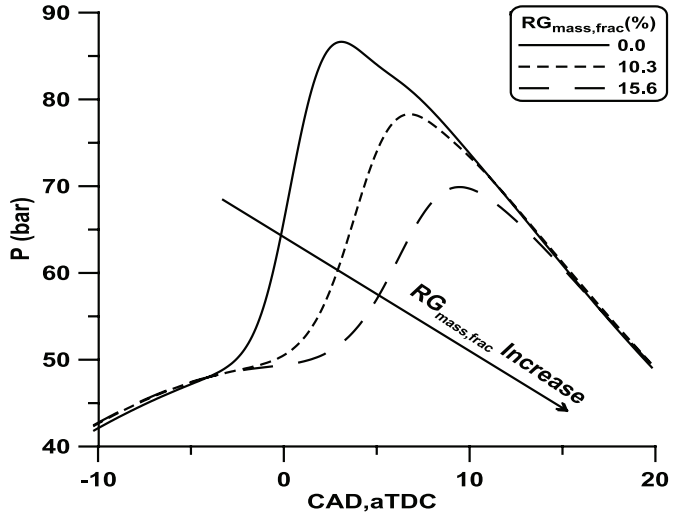

Fig. 11. Effect of RG on iso-Octane HCCI combustion pressure trace at constant λ and EGR, for group C cases of fixed EGR/λ indicated in TABLE 3

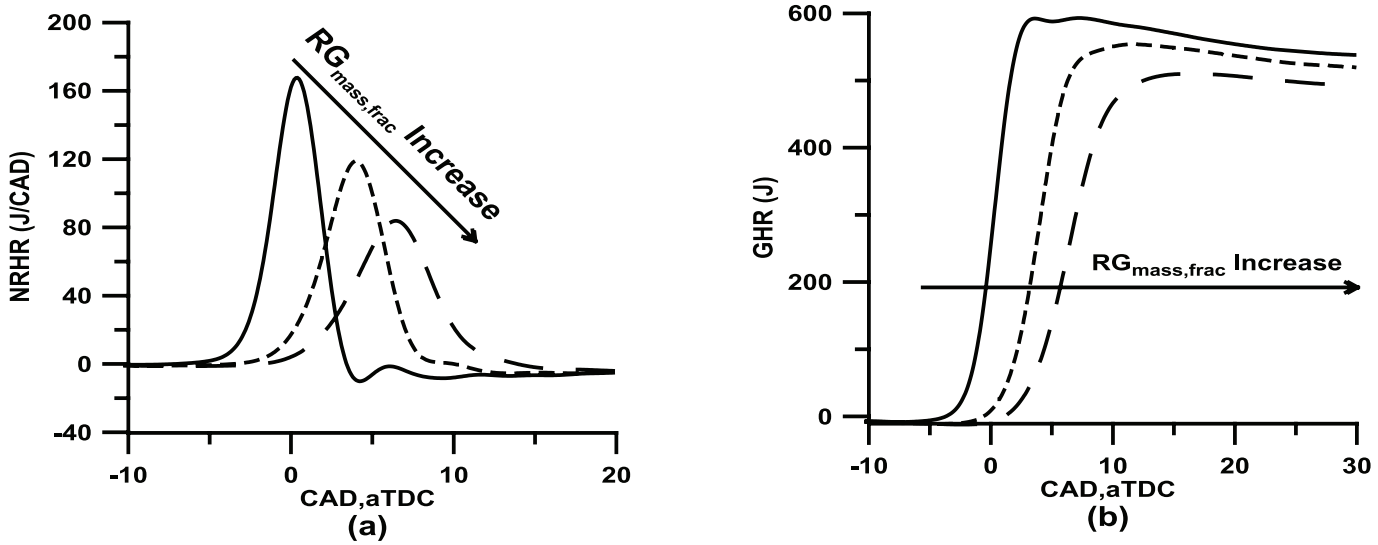

Fig. 12. Effect of RG on (a) net rate of heat release, and (b) gross accumulative heat release, iso-octane HCCI combustion for group C cases of fixed EGR/λ indicated in TABLE 3

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5.3 Iso-Octane base fuel discussion

ChemComb chemical kinetic simulations were not available for iso-octane so this discussion for the iso-octane case relies on experimental results and findings of other studies. In general, RG acted as a higher-octane blending agent and increasing RG blend fraction retarded ignition timing for the conditions tested here. However, the effect of RG on HCCI combustion of iso-octane is somewhat complex and differing results have been reported. In [23] Hosseini and Checkel showed only negligible effects of RG blending for iso-octane base fuel with a naturally aspirated HCCI engine. For these conditions, the CFR engine had a very narrow operating range between knock and misfire. For the same engine, adding 20% n-heptane to make a PRF80 base fuel intensified the RG effects which were to retard the HCCI combustion. As explained more in [23], HCCI ignition of high-octane fuels was dominated by temperature rather than pre-flame chemistry at the conditions set by naturally aspirated HCCI operation. Those results were similar with the findings of Eng et al (2002) [21] who showed a weak advance of ignition timing with RG blending.

In the current supercharged case, the initial conditions were more beneficial for HCCI ignition, providing more possibilities for chemical kinetics to be the governing factor. Our conclusion for high octane fuels like iso-octane is that, if the after-compression temperature is high (due to high intake temperature and/or high compression ratio), RG blending will affect combustion initiation through thermodynamic effects on end-of-compression temperature. RG blending increases mixture specific heat ratio, post -compression temperature is increased and combustion advances with RG enrichment similar to the case with natural gas. If the post-compression temperature is lower or the fuel has significant double-stage combustion behavior, (due to the presence of something like n-heptane in the fuel), the chemistry dictates the combustion initiation and RG blending will retard ignition timing. The balance between chemistry and thermodynamic effects determines whether the combustion timing will advance, retard or be un-affected by RG blending. From this point of view, RG blending is not a suitable technique to control HCCI combustion of iso-octane and may be of limited value with other fuels of similar octane rating.

6. Effect of RG on n-Heptane HCCI combustion

6.1 n-Heptane base fuel operating region

Compared with the high-octane fuels, HCCI combustion of n-heptane was relatively easy to achieve over a significant operating range using a moderate intake temperature and compression ratio. The strong double-stage combustion behavior of n-heptane. Fig. 13 shows the n-heptane HCCI combustion operating points with and without RG blending. RG blending with the n-heptane base fuel widened the operating range and shifted it towards leaner operation by providing more stable combustion with less misfire of lean mixtures.

Fig. 14 shows the relationships between λ, EGR and RG blending fraction. With n-heptane base fuelling, no limitation of RG blending ratio was observed at low or high λ or EGR values. As with the other fuels, sets of operating points with fixed λ and EGR values have been identified for further analysis and defined in TABLE 4.

TABLE 4. Selected groups of constant λ-EGR from n-heptane HCCI combustion operating region indicated in Error! Reference source not found.

Label	EGR(%)	λ
A	51.1	1.49
B	52.4	1.75
C	52.0	2.19
D	31.4	2.31
E	30.9	2.98
F	21.1	2.98

6.2 n-Heptane base fuel heat release characteristics

Fig.14 shows the effect of RG blending on HCCI combustion timing with n-heptane base fuel. Keeping other influential parameters constant, increasing RG blend fraction significantly retarded ignition timing. This effect was essentially linear with RG blend fraction and more than 10 CAD retard was possible using a 30% RG mass fraction. There was only a weak effect on combustion duration which was perhaps slightly prolonged by RG blending under some conditions.

Further detailed analysis of heat release patterns as shown in Fig. 15 indicates that increasing RG blend fraction prolonged the period between first-stage ignition and main combustion, (often called the negative temperature coefficient period), while reducing the ratio of the first to second stage combustion.

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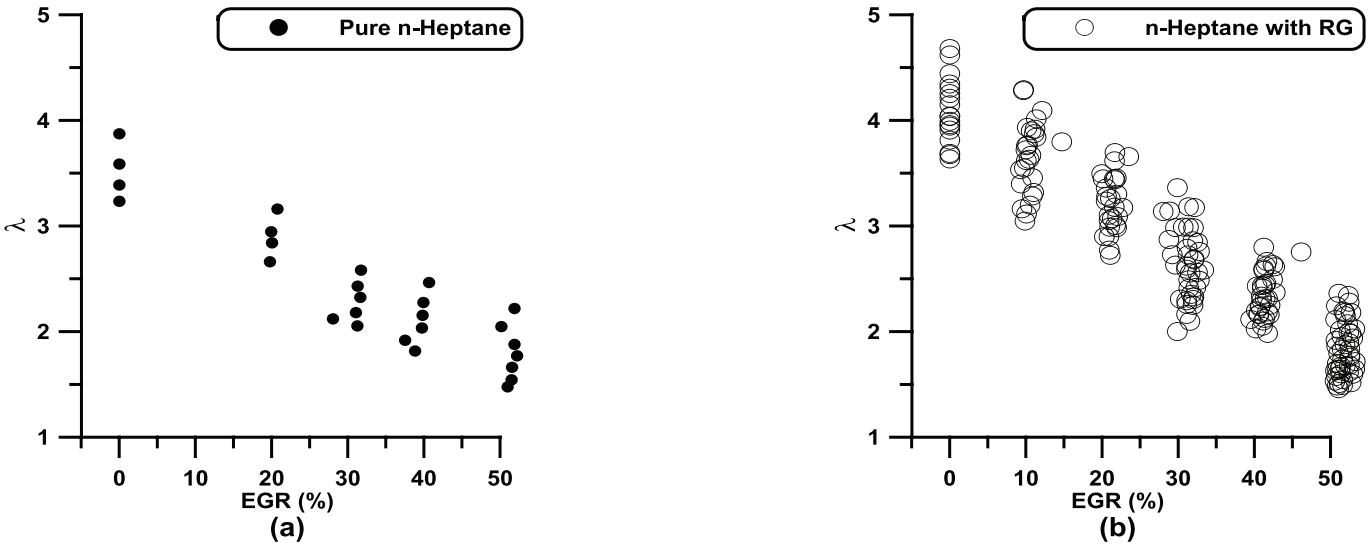

Fig. 13. λ-EGR operating region of n-Heptane HCCI combustion (a) pure n-Heptane and (b) n-Heptane enriched with RG

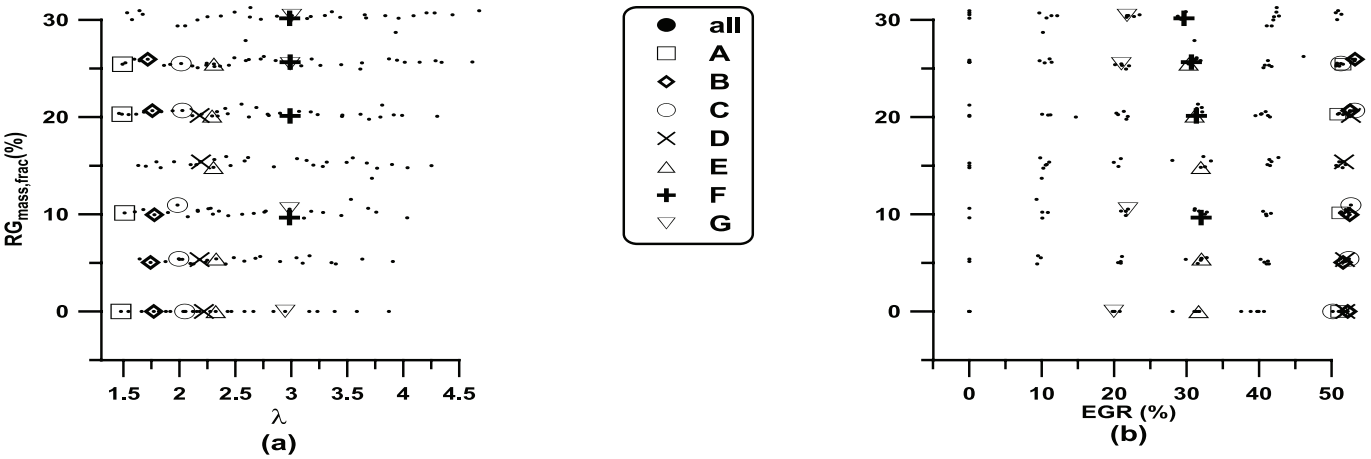

Fig. 14. (a) RG-λ and (b) RG-EGR operating regions for n-Heptane supercharged HCCI with indication of constant λ-EGR groups of data defined in TABLE 4

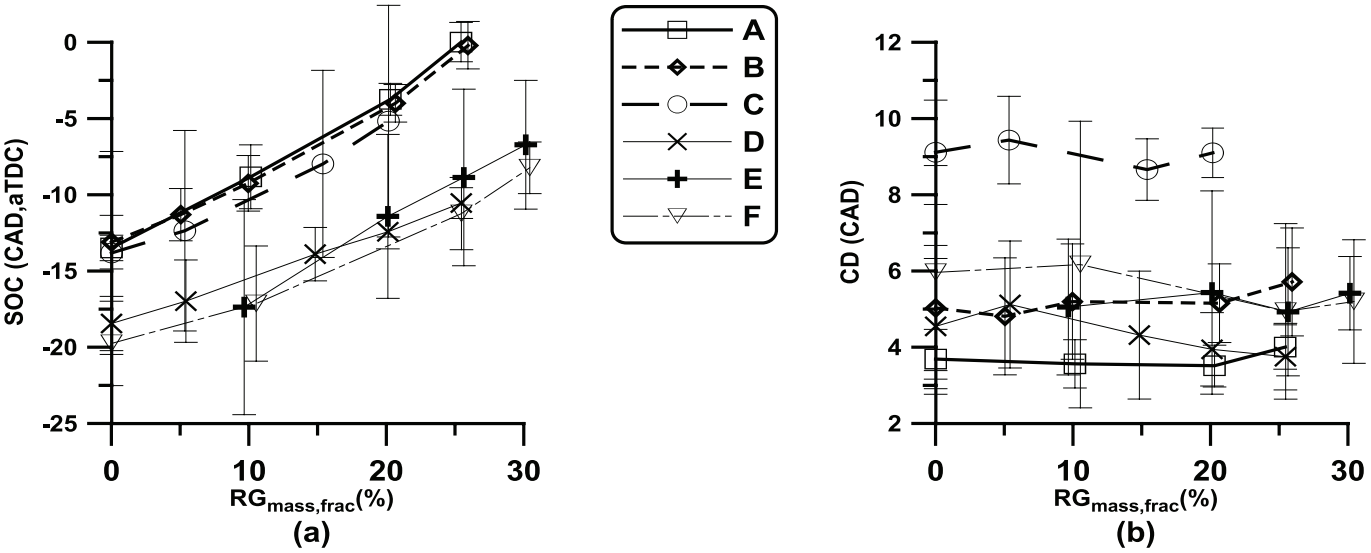

Fig. 15. Effect of RG on (a) start of combustion, and (b) combustion duration, HCCI combustion of n-heptane for selected constant λ-EGR cases of TABLE 4

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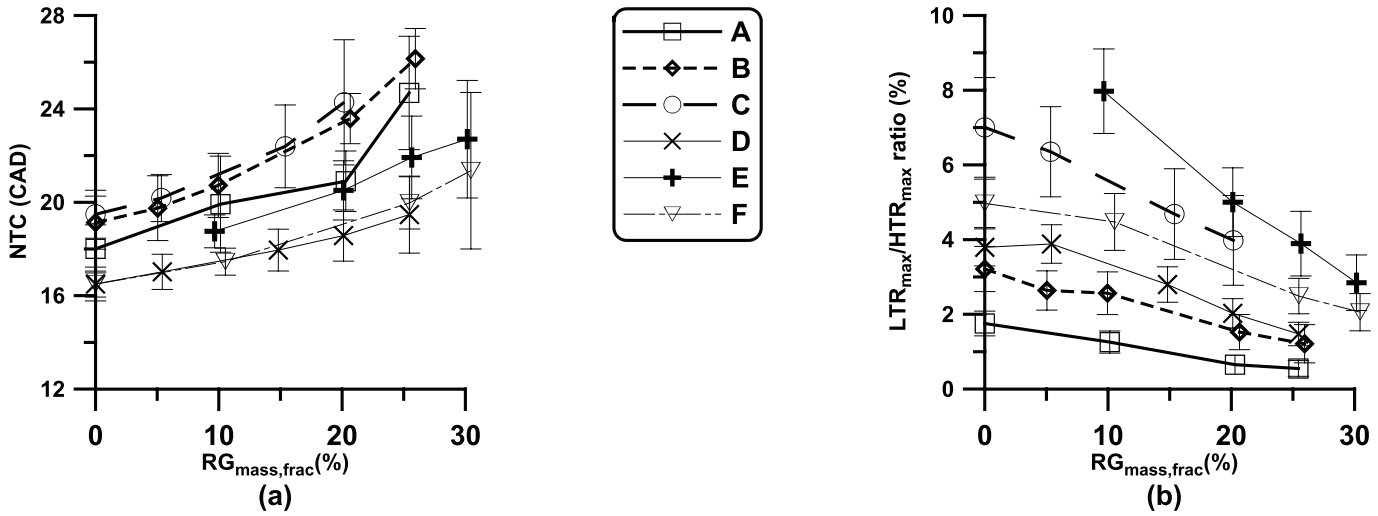

Fig. 16. Effect of RG on (a) negative temperature coefficient length, and (b) ratio of low to high temperature maximum rate of heat release, HCCI combustion of n-heptane for selected constant λ-EGR cases of TABLE 4

Fig. 16 shows the effect of RG on n-heptane HCCI combustion pressure traces for group B of the constant λ-EGR cases indicated in TABLE 4. With constant λ and EGR, increasing the RG blend fraction postponed the pressure trace, reducing maximum cylinder pressure and maximum pressure rise rate.

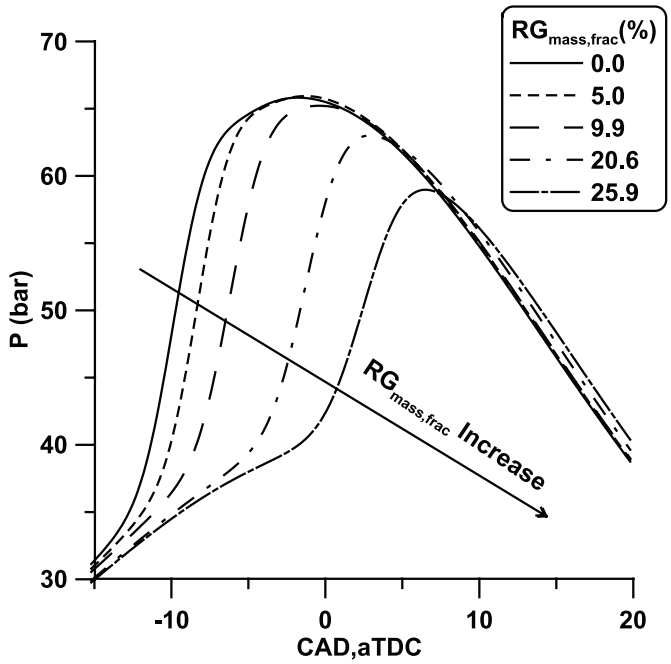

Fig. 17. Effect of RG on n-heptane HCCI combustion pressure trace at constant λ and EGR, for group B of data indicated in TABLE 4

Fig. 18 shows the effect of RG blending on net heat release rate and gross accumulative heat release for data group B of TABLE 4. In Fig. 17-a the first stage of heat release is magnified to show the significant effect of RG blending which decreases the magnitude of first-stage heat release and significantly delays the main heat release stage.

Increasing RGmass,frac, suppressed the first stage of heat release and consequently retarded the main stage of combustion as shown in both Fig. 17-a and –b.

6.3 n-Heptane base fuel modeling results

The effect of RG blending on n-heptane HCCI combustion was simulated using the ChemComb-SZM software, (see Kongsereeparp and Checkel (2007) [31] for validation). Fig. 19 shows the simulation results for a series of constant λ and EGR points at conditions similar to Fig. 18. The graph shows RG blending effects of reducing first-stage heat release and delaying main stage heat release which are very similar to those found in the experiments.

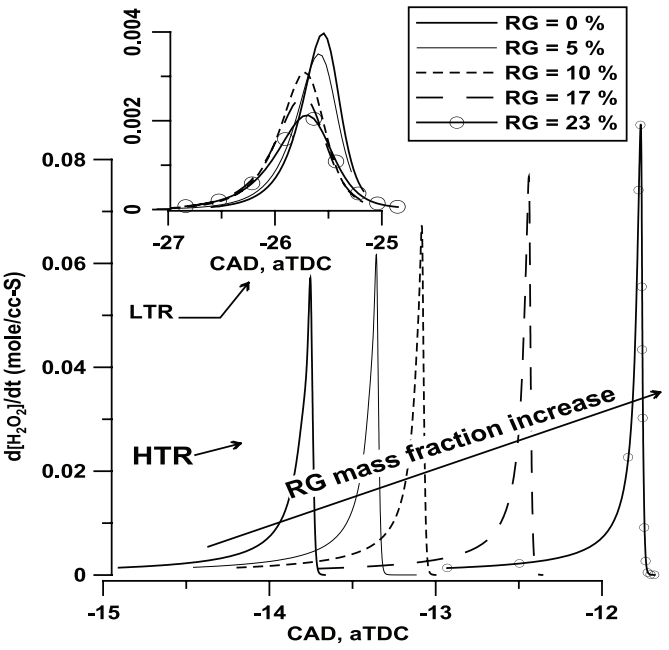

Fig. 19. Effect of RG on net rate of heat release for HCCI combustion of n-Heptane

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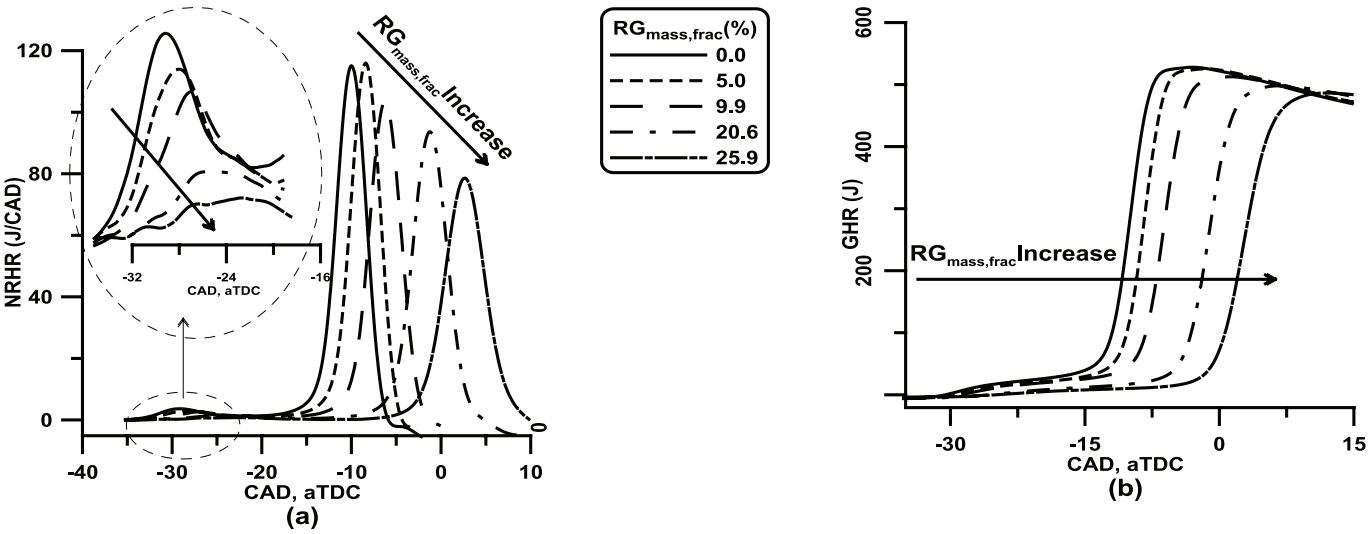

Fig. 18. Effect of RG on (a) net rate of heat release, and (b) gross accumulative heat release, n-heptane HCCI combustion for group C of data in TABLE 4

Fig. 19 shows an example of intermediate radical concentration drawn from the ChemComb model. Several species can be traced as indicators of the intermediate radical pool produced by pre-flame and cool-flame reactions. Hydrogen peroxide (H_2O_2) was chosen because it has a relatively large concentration, thus avoiding numerical uncertainty and is a significant participant in several chemical reaction paths. The rise of H_2O_2 concentration clearly indicates the first stage of combustion, the H_2O_2 concentration remains high through the negative temperature coefficient period, and then is consumed when the main stage of combustion initiates. Increasing RG blending fraction decreased the concentration of H_2O_2 between the two stages of combustion and is associated with a longer delay period between the first stage and the second stage.

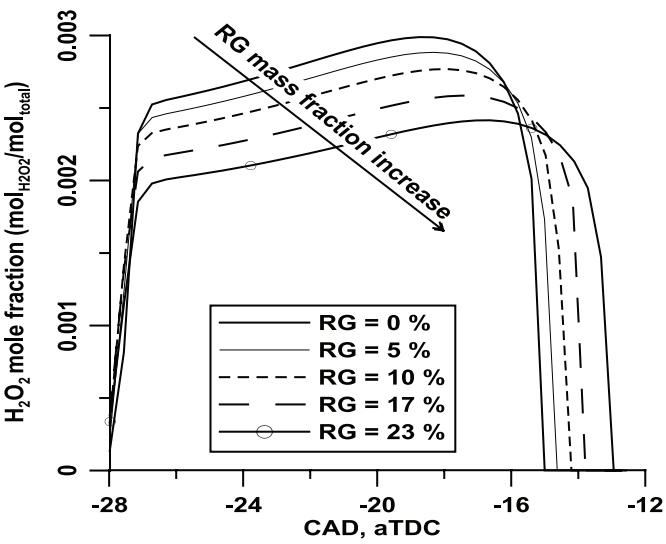

Fig. 20. Effect of RG on hydrogen peroxide concentration during NTC period, HCCI combustion of n-heptane at constant λ and EGR

6.4 n-Heptane base fuel discussion

Experimental and simulation results for this study of RG blending effects on HCCI combustion with n-heptane base fuel were in agreement with previous studies on fuels exhibiting two-stage combustion. Hydrogen is widely believed to act as a low temperature combustion suppressor and effectively to act as an octane number enhancer for conventional SI engine applications. In this case, blending hydrogen-rich RG effectively and progressively retarded HCCI ignition timing for all operating conditions tested with a base low-octane fuel. For the case of fuels with strong double-stage combustion, Hosseini and Checkel [24] have previously described using RG to effectively control HCCI combustion timing at constant λ and EGR (i.e. constant load). The capability to alter combustion timing without changing load makes RG blending an effective HCCI timing control mechanism. In most cases, optimized combustion timing could be obtained, resulting to optimum indicated power and thermal efficiency. The same observation of retarding HCCI ignition timing through RG blending was made by Shudo et al (2003) [14] for DME base fuelling. Also Eng et al (2002) [21] examined the effect of RG on n-heptane HCCI combustion and observed similar ignition retard behavior when HCCI combustion was enabled without exhaust re-breathing. In the case of exhaust re-breathing, combustion timing was not effectively altered by RG blending and this was attributed to ignition from hot internal residuals where the thermal condition dominated over the chemistry.

The simulation results confirmed the experimental observations. RG suppressed the first stage of combustion by competing to consume OH radicals with other reactions. The presence of H2, (and also with less effect of CO), effectively reduced the concentration of available free radicals produced by the

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first stage of combustion and this delayed the main combustion stage. Further, the enthalpy release from the first stage of combustion was reduced which had to be compensated by more time (or more compression) before the main stage combustion could occur.

7. Conclusions

RG blending was used to examine HCCI combustion timing control for three fuels of varying octane rating: natural gas, iso-octane and n-heptane. The fuels were tested in a CFR engine operated at steady state conditions with an intake heater and elevated intake pressure.

7.1 Natural gas

For the case of natural gas RG blending decreased the intake heating requirements, advanced combustion timing and reduced combustion duration. Chemical kinetic simulation showed the RG effects are dominated by thermal rather than chemical effects in this case. While natural gas HCCI combustion is difficult to achieve over a significant operating range, RG blending provides a predictable effect on HCCI ignition timing and might provide a means of HCCI timing control for natural gas engines.

7.2 Iso-Octane

With iso-octane fuel, RG blending retarded the combustion timing for the conditions tested. Differing effects of RG blending on iso-octane HCCI combustion timing have been found in studies at different operating conditions. We conclude that, with iso-octane fuel, the RG blending effect depends on the relative domination of thermodynamic and chemical kinetic effects at the specific operating conditions. When thermodynamic (compression temperature) effects dominate, RG blending will advance combustion timing. When chemistry (pre-flame reaction) effects dominate, RG blending will retard combustion timing. Because the effect of RG blending may vary with operating conditions, RG blending cannot be considered as a practical means of combustion timing control for fuels like iso-octane.

7.3 n-Heptane

The most attractive case for HCCI timing control through RG blending was found with n-heptane base fuel and this might be extended to any fuel which exhibits significant double-stage combustion behavior. RG could effectively control combustion timing over a significant range (more than 10 CAD) at constant EGR and λconditions corresponding to constant load. Simulation results confirmed that increasing RG blend fraction suppressed the low temperature heat release and postponed main stage of combustion by reducing the pool of intermediate radicals produced by the first stage combustion.

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