



Fuel reactivity as a means to control DI-HCCI combustion engine

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ABSTRACT

The homogeneous charge compression ignition (HCCI) is an advantageous combustion concept for internal combustion engines in terms of efficiency and pollutant emissions. This combustion strategy is one of the main types of low temperature combustion (LTC) concepts. It is a spontaneous multi-point combustion of a highly diluted premixed fuel-air mixture. However, its limited operating range suppressed its successful utilization. One applicable method to use this combustion concept in engines is to combine it with other combustion strategies while each combustion concept come into work during its optimum operating range. The idea of an HCCI combustion engine involving direct fuel injection into the combustion chamber is an applicable strategy aiming at this target. In the HCCI engines there is no direct control method for the time of auto-ignition. The octane number or fuel auto-ignitability characteristic is one of the most influential parameters on the combustion timing. Therefore, this study investigates the effect of the octane number on the direct injection (DI) HCCI combustion. The mathematical investigations are based on a novel two-stage combustion model. The combustion is predicted with the single-zone model from the intake valve closing to the end of injection. Thereupon, it is predicted by the multi-zone model. The results indicate that the octane number has profound effects on combustion phasing and delivered power. Therefore, cycle-by-cycle and cylinder-to-cylinder control of the combustion phasing by octane number adjustment is possible.



1) Introduction

Homogeneous Charge Compression Ignition (HCCI) combustion mode proposed by Onishi *et al.* [1] is a reliable method that has been found to produce ultra-low levels of nitric oxides and near zero soot emissions and to provide equal or greater fuel conversion efficiencies compared to that of the conventional direct injection (DI) diesel combustion [2-4].

The advantages of the HCCI combustion are commonly associated with its nature being a spontaneous multi-site combustion of a very lean and premixed fuel-air mixture which has high heat release rate and no significant evidence of flame propagation [4-7]. The high efficiency is due to the ability of operating with high compression ratios, lack of throttling losses at part load, lean combustion, and close to constant volume ideal Otto cycle heat release. However, there are some deficiencies intrinsic to the HCCI combustion which should be overcome [4-7]: The lack of any direct control method for the combustion timing; producing high levels of unburned hydrocarbons and carbon monoxide emissions; obtaining an appropriate fueling rate for achieving high engine loads under mechanical limitations of engine.

In order to make the HCCI engine a feasible alternative to the conventional engines, several items must be elucidated. Control of the combustion timing is one of the most important of these items to be resolved. The combustion timing should be controlled in order that heat is released at the best time in the engine cycle.

The HCCI combustion is a form of natural auto-ignition. Thus it is highly sensitive to the mixture's thermal, physical and chemical properties. The intake temperature, pressure, air/fuel ratio, auto-ignitability, and exhaust gas recirculated (EGR) rate are the most influential parameters.

It is arguable that the auto-ignitability of mixtures used in an HCCI engine should be defined as a function of octane number (ON), temperature history and other factors [8-12]. However, the ON alone is still a good and easy approximation of the auto-ignitability of fuel mixtures in an HCCI engine [8]. Fuel mixtures having higher octane ratings are more difficult to auto-ignite. Since the ignition timing of HCCI engines depends on the auto-ignition of the in-cylinder charge, variable blends between two different octane fuels can significantly change the HCCI combustion behavior and the engine performance.

Studies show that at a given intake temperature, mixtures of lower ON fuels require lower intake temperature [11, 13] and could achieve a wider operating range [8, 14]. However, using low ON fuels could lead to the early ignition and therefore is applicable only to low compression ratio (CR) engines, thus reducing efficiency [8]. Using high ON fuels retards the combustion start, decreases the

combustion efficiency, increases HC-CO emissions [15], decreases NO_x emissions and requires hotter intake mixtures or greater CR [8]. Several attempts have been tried to control fuel qualities (in terms of ON) by blending two different fuels such as diesel/gasoline [16-18], heptane/ethanol [19, 20], heptane/butanol [21], dimethyl ether (DME)/methanol-reformed gas [22], DME/methanol [23], DME/methane [24], heptane/iso-octane [25-29], natural gas/heptane [7, 30], gasoline/hydrogen, and natural gas/hydrogen [31, 32]. Blends with reformed fuels have also shown significant effects on the HCCI combustion and therefore, have been demonstrated as a feasible means for the HCCI combustion timing control [5, 31, 33-35].

In [25-27, 29], dual fuel systems having fuels of two completely different auto-ignition characteristics, namely iso-octane and n-heptane are used to modulate ON for the combustion phasing control. Normal heptane is an easily self-ignited fuel whereas iso-octane is a more self-ignition resistant one. Therefore, different mixing ratios of these two fuels provide a wide range of auto-ignition properties which enables the combustion phasing control [12]. In terms of fuel injection consideration, it is agreed that injection timings typically before the piston has reached roughly two-thirds of its upward movement in the compression stroke [36] (i.e. the whole injection duration occurring before -60 crank angle degrees after top dead center (CAD, ATDC)) can be regarded as HCCI [37].

Therefore, the focus of this study is to investigate the influence of ON on DI-HCCI engine performance characteristics by a novel mathematical model developed by the authors [38]. In the following sections, the mathematical modeling is introduced first. Thereupon, the model setup is demonstrated. Afterwards, the results of applying the model to the determined operating points are discussed. Finally, conclusions from this study are explained.

2) Mathematical Modeling

The idea of the developed model by the authors [38] stems from the fact that in the DI-HCCI combustion regime (when the whole injection duration occurs before -60 CAD, ATDC), the effect of stratification caused by the direct fuel injection is not a highly influential factor [37]. The model uses Cantera [39] as the solver for chemical kinetics which yields the rate of production/consumption of species' mass fractions due to the reactions at each instance. Moreover, thermodynamic and transport properties of the in-cylinder mixture is obtained by Cantera at each time-step.

The combustion model [38] is a two stage one. In the first stage, a single-zone model predicts in-cylinder combustion behavior from the intake valve closing (IVC) to the end of injection (EOI). After EOI, the combustion chamber charge is a mixture of air, EGR,

and fuel. So, a multi-zone model is developed to predict in-cylinder charge behavior for the second stage from EOI to exhaust valve opening (EVO). The comparison between the experimental results and the model predictions revealed that the assumption of neglecting the injection-induced stratification is valid [38]. The model provided acceptable results which reveals its capability to adequately well capture DI-HCCI combustion engine performance. The average errors in the model prediction of the maximum in-cylinder pressure rise rate and the peak in-cylinder pressure are reported as 20 and 3%, respectively. Meanwhile, the combustion phasing is estimated with average error of 0.1 crank angle degrees. Whereas, the power is estimated with average error of 1%.

3) Model setup

The investigations are carried out on an engine with the specifications shown in Table 1 [38]. In this study, a binary mixture of n-heptane and iso-octane called primary reference fuel (PRF) is used.

Table 1: Engine specifications

Bore (mm)	130
Stroke (mm)	158
Compression ratio	15.7
Engine speed (rpm)	1200
IVC (CAD, ATDC)	-153
EVO (CAD, ATDC)	128

In order to investigate the influence of ON on DI-HCCI engine performance characteristics, ON sweep is performed. Two data-sets with two different intake charge temperatures, including 14 cases are studied in this evaluation. The investigation matrix of the two data-sets is demonstrated in Table 2. To avoid the influence of EGR, load, intake pressure, and injection timing on the performance of the DI-HCCI engine, they are kept constant.

Table 2: Investigation matrix based on octane number sweep

	data-set I	data-set II
Injected fuel mas per cycle (mg)	42.5	42.5
EGR (%)	44	44
IVC Pressure (bar)	1.37	1.37
Start of Injection (CAD, ATDC)	-90	-90
Intake temperature (K)	340	346
ON sweep	67-73	67-73

The first stage of the simulation from IVC to EOI is analyzed with a single-zone model, and the second stage from EOI to EVC is analyzed using the multi-zone approach. The initial conditions for the multi-zone period are set from the results at EOI from the

single-zone model. The zonal temperatures are assumed to be identical at EOI timing. The in-cylinder temperature gradient is formed during the compression after EOI due to the work and the heat transfer between zones. One further model input is the chemical kinetics mechanism. In this study of PRF-fueled DI-HCCI combustion engine a 171-species mechanism for PRF [40] is used.

4) Results and Discussion

The influence of ON changes on the combustion timing of the studied DI-HCCI engine in terms of the crank angle when half of the fuel is burnt (CA50) is demonstrated in Figure 1 for the two data-sets. As ON increases the fuel becomes more resistant to the auto-ignition, thus the auto-ignitability reduces. It is seen that increasing ON retards the combustion timing. As aforementioned, it is generally accepted that the combustion in HCCI engines is controlled by chemical kinetics. Thus, higher ON which means lower auto-ignitability leads to later combustion phasing. Furthermore, it is seen in Figure 1 that higher intake charge temperature of data set II results in advanced combustion timing. Higher charge temperature makes the in-cylinder mixture overcome the threshold energy earlier.

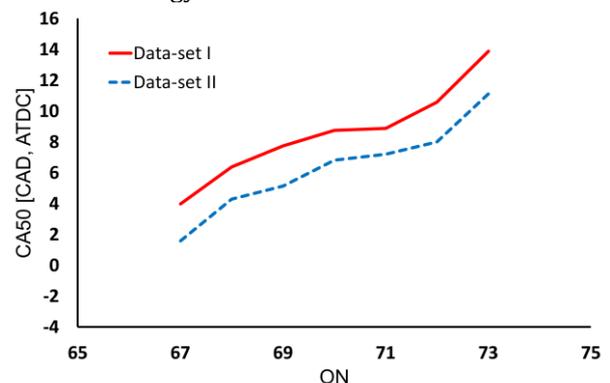


Figure 1: The influence of ON variation on combustion phasing

The influence of ON variation on the characteristics of the in-cylinder pressure for the two data-sets is demonstrated in Figure 2 and Figure 3. As aforementioned, one of the challenges of the HCCI combustion engine operation is the limitations in the operating range due to misfire and knock. Maximum pressure rise rate can be considered as a measure of combustion severity and/or knock [38]. Figure 2 illustrates the results of the peak in-cylinder pressure and Figure 3 demonstrates the maximum amount of the pressure rise rate. The results indicate that increasing ON leads to lower peak pressure and maximum pressure rise rate. The reduction in the pressure rise rate is a means to avoid the incidence of knocking. Therefore, there is a compromise between the benefits of the combustion phasing adjustment by ON modulation and the mechanical limitations of the engine structure in the case of lowering ON.

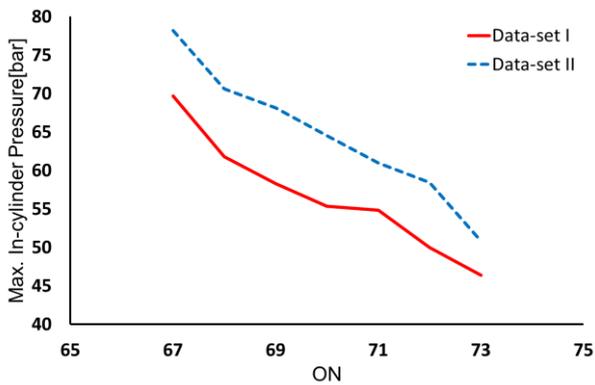


Figure 2: The influence of ON variation on the peak in-cylinder pressure

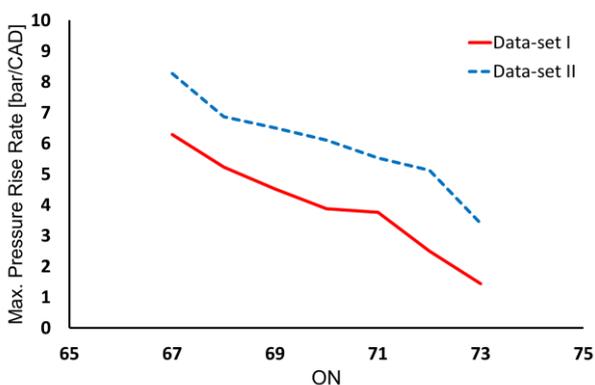


Figure 3: The influence of ON variation on the maximum in-cylinder pressure rise rate

Indicated mean effective pressure (IMEP) is a proxy for the delivered power of an engine. It is defined as the indicated work output per unit of the engine swept volume. IMEP is calculated for each individual cycle using the in-cylinder pressure trace. Since in this study only the closed part of the cycle is modeled, gross IMEP is investigated. Figure 4 illustrates the gross IMEP with respect to ON for the two data-sets. In higher ON, lower power output and density are achieved due to the lower peak pressure and maximum pressure rise rate which result in the decreased IMEP.

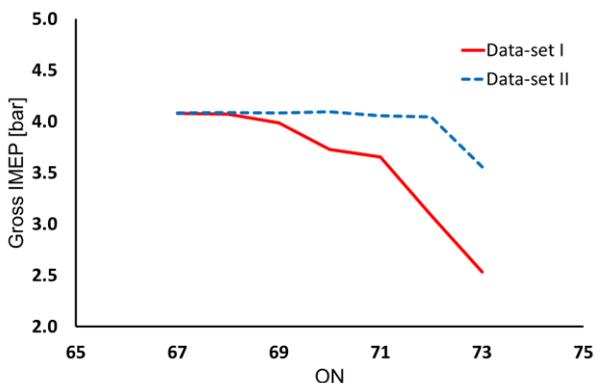


Figure 4: Gross IMEP vs. ON for two data-sets

Figure 5 and Figure 6 depict in-cylinder mean charge temperature calculated from the developed model for data-set I and data-set II, respectively. As can be seen, combustion temperature increases with increased fuel auto-ignitability (decreased ON). Peak in-cylinder mean charge temperature follows peak in-cylinder mean charge pressure trend of Figure 2 and Figure 3, and generally increases by increasing fuel auto-ignitability. The advanced combustion phasing of the cases with lower ON as demonstrated in Figure 1 enhances peak temperature of the in-cylinder charge.

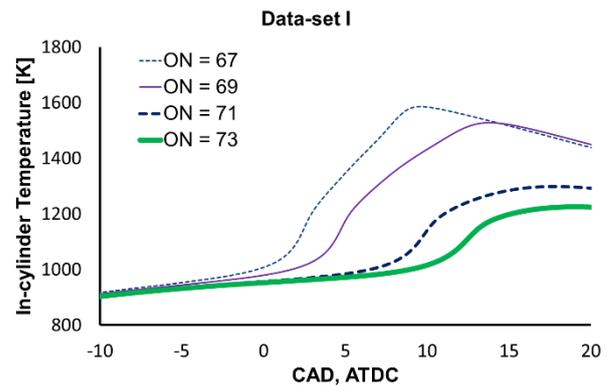


Figure 5: Calculated in-cylinder mean charge temperature for data-set I

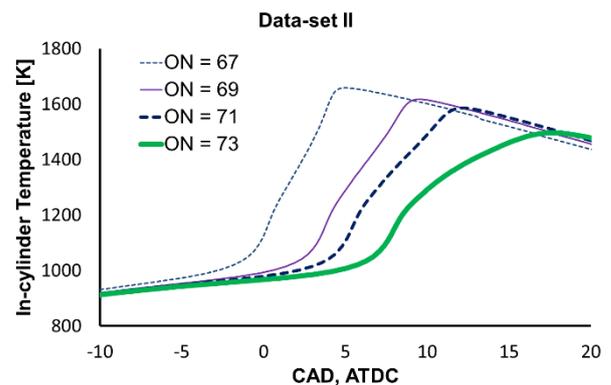


Figure 6: Calculated in-cylinder mean charge temperature for data-set II

The calculated apparent heat release rate for the investigated cases of data-set I and data-set II are shown in Figure 7 and Figure 8, respectively. As can be seen, the variation of fuel auto-ignitability by changing the ON of the fuel mixture has profound effects on heat release rate magnitude and phasing. Increased auto-ignitability results in advanced combustion (closer to TDC) which therefore leads to an increase in the maximum heat release rate. The phasing of heat release rate curves is consistent with the results of combustion phasing parameter which advances with reduced ON.

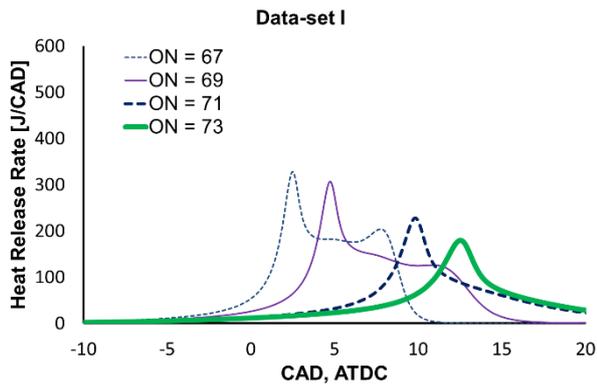


Figure 7: The effect of ON variation on apparent heat release rate for data-set I

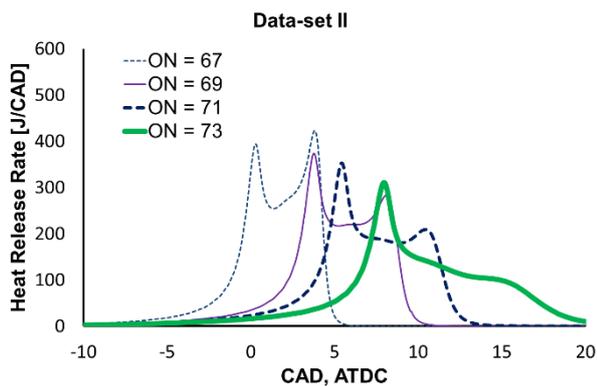


Figure 8: The effect of ON variation on apparent heat release rate for data-set II

As discussed previously, altering the fuel auto-ignitability affects the in-cylinder charge pressure trace. The pressure traces for two data sets are illustrated in Figure 9 and Figure 10. Peak pressure location affects its magnitude. As can be seen from the figures, the peak pressure continues to decrease due to retardation of its location. The delayed combustion phasing leads to a decrease in maximum in-cylinder charge pressure.

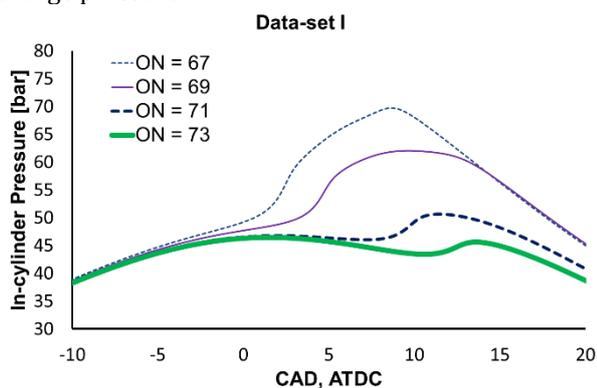


Figure 9: Calculated in-cylinder pressure traces for data-set I

Conclusions

In this study, the effect of ON variation on the DI-HCCI combustion engine performance characteristics is investigated. The investigations are based on a novel

two-stage thermo-kinetic model. The findings of the present study can be summarized as follows:

- The combustion phasing alters with the ON variation. The combustion timing is delayed due to the increased ON.
- Increasing ON generally reduces the peak cylinder pressure and the pressure rise rate during combustion.
- Increasing ON reduces the gross IMEP.
- It is possible to perform the cycle-by-cycle and cylinder-to-cylinder control of the combustion phasing of the DI-HCCI combustion engine by octane number adjustment.

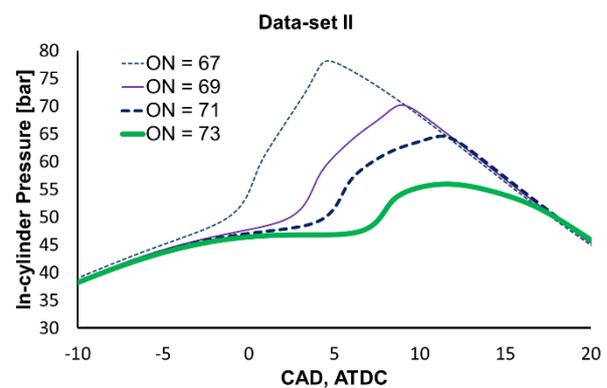


Figure 10: Calculated in-cylinder pressure traces for data-set II

List of Symbols – Abbreviations

ATDC	after top dead center
CAD	crank angle degrees
CA50	crank angle when half of the fuel is burnt
CR	compression ratio
DI	direct injection
EGR	exhaust gas recirculated
EOI	end of injection
EVO	exhaust valve opening
HCCI	Homogeneous charge compression ignition
IVC	intake valve closing
ODE	ordinary differential equation
ON	octane number
PRF	primary reference fuel
SOI	start of injection

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واکنشگری سوخت، راهکار تنظیم موتور اشتعال تراکمی بار همگن با پاشش مستقیم

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زمانبندی احتراق

تنظیم (کنترل)

احتراق اشتعال تراکمی بار همگن، یک مفهوم احتراقی مفید، از نظر بازدهی و میزان آلاینده‌های منتشره، برای موتورهای درون‌سوز است. این راهبرد احتراقی، یکی از مهمترین انواع احتراق کم‌دما سوز است. این شیوه، احتراق هم‌زمان حجمی مخلوط پیش-آمیخته بسیار رقیق سوخت و هوا است. لیکن بازه کارکردی محدود این نوع احتراق سبب شده است که استفاده کاربردی از آن در موتورها تاکنون موفق نبوده باشد. یکی از روش‌های کاربردی نمودن این نوع احتراق در موتورها این است که با دیگر انواع احتراق ترکیب گردد و هر نوع از احتراق در بازه کارکردی بهینه خود ایفای نقش نماید. ایده موتور اشتعال تراکمی بار همگن که در آن تزریق مستقیم سوخت به داخل محفظه احتراق انجام می‌شود راهبرد مناسبی برای نیل به این هدف می‌باشد. در موتورهای اشتعال تراکمی بار همگن ابزار کنترلی خارجی که مستقیماً زمان خوداشتعالی را تنظیم نماید وجود ندارد. عدد اکتان یا میزان واکنشگری سوخت یکی از اثرگذارترین پارمترها بر زمانبندی احتراق است. بنابراین، این پژوهش به بررسی اثر عدد اکتان سوخت بر احتراق اشتعال تراکمی بار همگن با پاشش مستقیم سوخت به محفظه احتراق می‌پردازد. بررسی‌های ریاضی بر مبنای یک مدل احتراقی جدید دو مرحله‌ای است. پیشبینی احتراق، از زمان بسته شدن دریچه هوا تا پایان پاشش سوخت با مدل تک منطقه‌ای، و از آن پس تا زمان باز شدن دریچه دود، با مدل چندمنطقه‌ای اجرا می‌شود. نتایج نشان می‌دهند که عدد اکتان اثر چشمگیری بر زمانبندی احتراق و توان تولیدی دارد. بنابراین، کنترل چرخه-به-چرخه و استوانه-به-استوانه زمانبندی احتراق با تنظیم عدد اکتان سوخت قابل اجرا خواهد بود.



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