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Simulation of predictive kinetic combustion of single cylinder HCCI engine

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Abstract. Homogeneous Charge Compression Ignition (HCCI) engine has attracted great attention due to its improved performance and emissions compared to conventional engines. It can reduce both Nitrogen Oxides (NOx) and Particulate Matter (PM) emissions simultaneously without sacrificing the engine performance. However, controlling its combustion phasing remains a major challenge due to the absence of direct control mechanism. The start of combustion is entirely initiated by the chemical reactions inside the combustion chamber, resulted from the compression of its homogeneous mixtures. Varying some critical engine parameters can play a significant role to control the combustion phasing of HCCI engine. This paper investigates the characteristics of HCCI combustion fuelled with n-heptane (C_7H_{16}) using single-zone model computational software. The model enabled the combustion object to vary from cycle to cycle. Detailed simulations were conducted to evaluate the effects of air fuel ratio (AFR), compression ratio (CR) and intake air temperature on the in-cylinder pressure and heat release rate. The simulation results showed that the single-zone model was able to predict the two-stage kinetic combustion of HCCI engine; the Low Temperature Heat Release (LTHR) and the High Temperature Heat Release (HTHR) regions. It was found that minor changes in AFR, CR and inlet air temperature led to major changes in the HCCI combustion phasing.

1. Introduction

One of new combustion technologies that attracts numerous attention is Homogeneous Charge Compression Ignition (HCCI) engine. It combines the best features of both Spark Ignition (SI) and Compression Ignition (CI) engines, offering a relatively high efficiency with low Nitrogen Oxides (NOx) and Particulate Matter (PM) emissions [1]. The homogeneous mixture is achieved without using spark plug or injector to control its combustion phasing [2]. Due to the absence of additional equipment to regulate its start of combustion, an HCCI engine does not typically give large gradients of spatial temperature from the flame front [3]. As a result, it can significantly reduce NOx emissions. Moreover, since the mixture is premixed and very lean, it creates homogeneous charges inside the cylinder thus reducing the PM emissions significantly [4]. In addition to its low emissions characteristic, an HCCI engine can also be operated at high compression ratio, producing more power and achieving higher efficiency compared to conventional engines [5].

However, despite its benefits in terms of high performance and low emissions, the combustion of HCCI engine is difficult to control [6]. Conventional engines such as SI and CI engines use external devices i.e. spark plug in SI engine or injector in CI engine to control the start of combustion. In HCCI engine, such devices are not available. Moreover, to be widely used as a commercial engine, the HCCI technology has still a number of challenges to be solved. These include narrow operating range and the difficulty to regulate its heat release rate [2]. It is also important to note that as the mixtures between air and fuel ignite nearly simultaneously at multiple location within the cylinder, knocking and misfire phenomena may occur [7]. Therefore, controlling the combustion phasing remains the biggest challenge in HCCI combustion.

Since no external source of energy is used to control its ignition timing, the auto-ignition depends entirely on the chemical kinetics and combustion environment within the cylinder [8]. Changes in the cylinder environment can affect the combustion phasing of HCCI engine [9]. Varying the air fuel ratio (AFR), intake air temperature and compression ratio (CR) have the potential to assist the combustion control of HCCI engine [10]. However, if the value of these engine parameters reach to a point where the rich mixtures are created inside the combustion chamber, the early auto-ignition may occur which eventually cause knocking [11]. On the other hand, if too lean mixtures are formed, misfire and incomplete combustion may take place, increasing the unburned Hydrocarbons (uHC) and Carbon Monoxide (CO) emissions of HCCI engine [12]. Thus, further investigation is needed to understand the optimised operating range of HCCI for various AFR, CR and intake air temperatures.

To investigate the combustion behaviour of an HCCI engine, it is important to have the right fuel and its chemical mechanism. Commercial diesel fuel contains a mixture of alkanes, aromatics, cycloalkanes and olefins [13]. Consequently, it is difficult to understand its chemical mechanism due to its oxidation complexity of all the chemistry compounds. Unlike diesel fuel in the market, surrogate mixture such as n-heptane is free from aromatics and has higher volatility as well as less sulfur content compared to diesel fuel. Therefore, n-heptane is often used as the primary reference fuel (PRF) to substitute commercial diesel fuel in numerous studies. It is suitable to be operated in HCCI as the cetane number of n-heptane is comparable to commercial diesel fuel [14]. As a result, the combustion characteristics of both fuels are almost similar due to its identical cetane number [15].

Given the costly nature of experimentation using engine test bench, simulation work using computer programme is often preferred. A simulation model can provide insight into the effect of different parameters by isolating some of their values [16]. Various simulation models have been proposed [17–20]. In general, the models can be grouped into two categories; chemistry model and fluid dynamic model [20]. The chemistry model, also referred to as the zone model, takes into account the chemical reaction in the cylinder using detailed kinetic mechanism. The fluid mechanics and heat transfer phenomena are simplified in this model. On the other hand, in the second model, focus is given on the fluid dynamic and heat transfer phenomena. The fluid dynamic model is usually performed using Computational Fluid Dynamics (CFD) with chemical reaction being simplified. Considering that HCCI combustion is primarily governed by chemical kinetics and less influenced by the fluid mechanics or heat transfer phenomena, the zone model is preferred in the simulation of HCCI combustion.

The zone model is normally classified into the single-zone and the multi-zone models [21]. The single-zone model does not require high performance computing process as it neglects the temperature and the inhomogeneity of the composition inside the cylinder. The combustion duration is underestimated, while the pressure peak is overestimated [22]. Therefore, it cannot predict accurately a number of extreme conditions such as high Exhaust Gas Recirculation (EGR) or very lean mixture, owing to the neglection of the temperature and the inhomogeneity of the mixtures. On the other hand, the multi-zone model takes into account both the temperature and the inhomogeneity. It enhances the idea of single-zone model by dividing the cylinder volume into several zones with each zone having its own characteristics of temperature and composition [23]. Multi-zone models may slightly be different with one another due to the variation between the interaction of one zone with its neighboring zone.

Fiveland and Assanis [24] developed a single-zone model to investigate the performance and combustion of HCCI engine fuelled with hydrogen or methane. The effects of AFR, CR, and inlet temperature were investigated. It was found that the development of mixture preparation and ignition point significantly affected the volumetric efficiency and power output. They concluded that HCCI operation fuelled with natural gas needed high compression ratios as well as low intake temperatures to promote the auto-ignition. In terms of the fuel, previous studies have shown that the operating region of HCCI engine fuelled with n-heptane is extremely narrow due to early ignition and knock problem at lower AFR. Hasan et al. [4] used a single zone model to evaluate HCCI combustion and performance using a reduced n-heptane chemical reaction mechanism. The model was successful in capturing the combustion phasing of HCCI engine, particularly the Low Temperature Heat Release (LTHR) region, for different AFR, CR, engine speed, inlet air temperature and intake air pressure. It was found that the combustion was advanced and the combustion duration was shortened with the increase of the intake air temperature and the decrease of the engine speed.

Previous studies mentioned above have indicated that the problem in HCCI combustion phasing could be effectively controlled by changing a number of engine parameters using computational programme. Fathi et al. [23] investigated both the single-zone and multi-zone approaches in the HCCI combustion modelling. It was found that the single-zone model gave over-prediction on the in-cylinder pressure. Moreover, the maximum pressure rise rate was also significantly overestimated. On the other hand, the multi-zone model provided better predictions on the combustion phasing and the maximum pressure rise rate. However, the use of multi-zone model requires significant amount of time and resources. This study indicated that if the initial conditions were set properly and the heat transfer during the compression stroke was carefully estimated, the start of main combustion could be predicted accurately using single-zone model.

To take the advantage of speed and low cost of computational study, this paper aims to develop a simulation model of HCCI engine fuelled with n-heptane using single-zone model to vary the combustion object from cycle to cycle. The combustion analysis was carried to evaluate the in-cylinder pressure and heat release rate for various air-fuel ratios, compression ratios and intake air temperatures.

2. Methodology

Figure 1 shows detail of the entire model from the inlet part to the engine and exhaust system. The specifications of the engine cylinder geometry are as follows; bore = 86 mm, stroke = 86.07 mm, connecting rod length = 175 mm, and TDC clearance height = 1 mm.

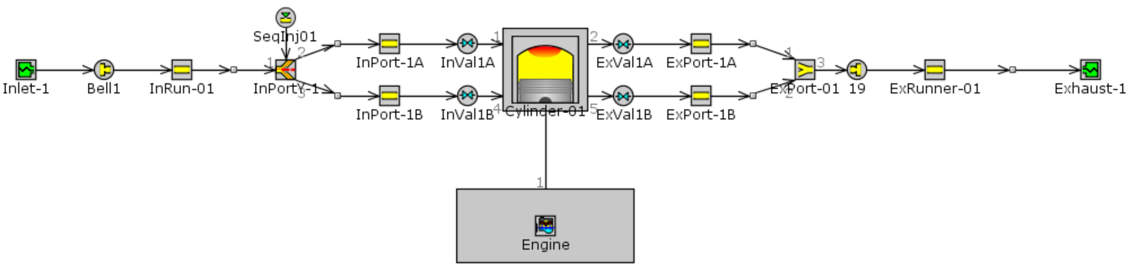

Figure 1. Schematic diagram of the model

The Woschni GT model was used to estimate the heat transfer in the cylinder. This is a modified model from classical Woschni in which the coefficients of heat transfer are obtained when the valves are open. As a result, the Woschni GT model is more accurate since it considers the increase of heat transfer resulted from the inflow velocities at the intake and the backflow velocities at the exhaust valve. Furthermore, the modelling was performed in a perfectly mixed zone using one-dimensional engine modelling software. The injector delivery rate was set to 7 g/s with 360 degree injection timing angle and 0.3 vaporized fluid fraction. The model allowed the combustion object to vary from cycle to cycle. As a result, this mixed-mode model could be used at different cycles during the same transient simulation for HCCI model.

To understand the use of n-heptane in HCCI engine for a wide range of operating conditions, varying some engine parameters such as air-fuel ratio (AFR), compression ratio (CR) and intake air temperature were needed. Firstly, the value of AFR was varied between 30 and 50, while intake air temperature, pressure, CR, EGR and engine speed were kept constant. Afterwards, the value of CR was varied between 10 and 16. Lastly, the intake air temperature was varied between 300 and 360 K, while other engine parameters such as AFR, CR, EGR and engine speed were kept constant. Table 1 provides the simulation matrix of the parameters and variables used in the simulation.

Table 1. Simulation matrix

No.	AFR	CR	Intake Air Temperature (K)	Pressure (bar)	EGR (%)	Speed (rpm)
1.	30-50	10	325	1	20	1000
2.	45	10-16	325	1	20	1000
3.	45	10	300-360	1	20	1000

The values presented in Table 1 are sufficient to achieve the HCCI combustion. As mentioned in the introduction, HCCI is limited by its narrow range of operation. At rich mixtures, early auto-ignition may occur resulted from its high in-cylinder pressure and temperature that eventually leads to knocking. At too lean mixtures, the auto-ignition cannot be achieved thus creating incomplete combustion and misfire. Therefore, the selection of variables and constant parameters is of great importance in engine simulation. The values given in the simulation matrix above are within the accepted operating range to achieve the HCCI combustion [4].

3. Results and discussion

The use of conventional diesel fuel or n-heptane in HCCI engine tends to produce a two-stage heat release region; the Low Temperature Heat Release (LTHR) and the High Temperature Heat Release (HTHR). This two-stage heat release characteristic is also observed in other diesel-like fuels such as straight carbon-chain paraffin, Fisher-Tropsch naphtha and Dimethyl Ether (DME).

3.1. Effect of air-fuel ratio (AFR)

The HCCI combustion depends heavily on the homogeneous mixture to produce high efficiency and low emissions level. Varying the air fuel ratio is considered as the most practical approach to assist the homogenization of the mixture. Figure 2 shows the effect of various AFR on HCCI in-cylinder pressure. The value of AFR was varied between 30 and 50 for a constant intake air temperature (325 K), pressure (1 bar), CR (10), EGR (20%) and engine speed (1000 rpm).

Figure 2 shows that as the value of AFR increases, the in-cylinder pressure decreases and the peak pressure is retarded. As a result, longer combustion delay is observed with higher AFR (lean mixtures). On the other hand, low AFR has relatively shorter combustion delay as its high fuel composition increases the speed of its charge chemical reactions. As a result, the lowest AFR in the graph has the most advanced and highest peak pressure. However, the use of low AFR or rich mixtures may lead to excessive pressure and damage the engine due to its early auto-ignition and high peak pressure. To prevent these problems, higher amount of AFR or highly diluted mixture is required to lower the speed of chemical reactions so that extreme pressure can be avoided. Results from Figure 2 indicates that varying the value of AFR can be used as an effective method to control the in-cylinder pressure of HCCI combustion.

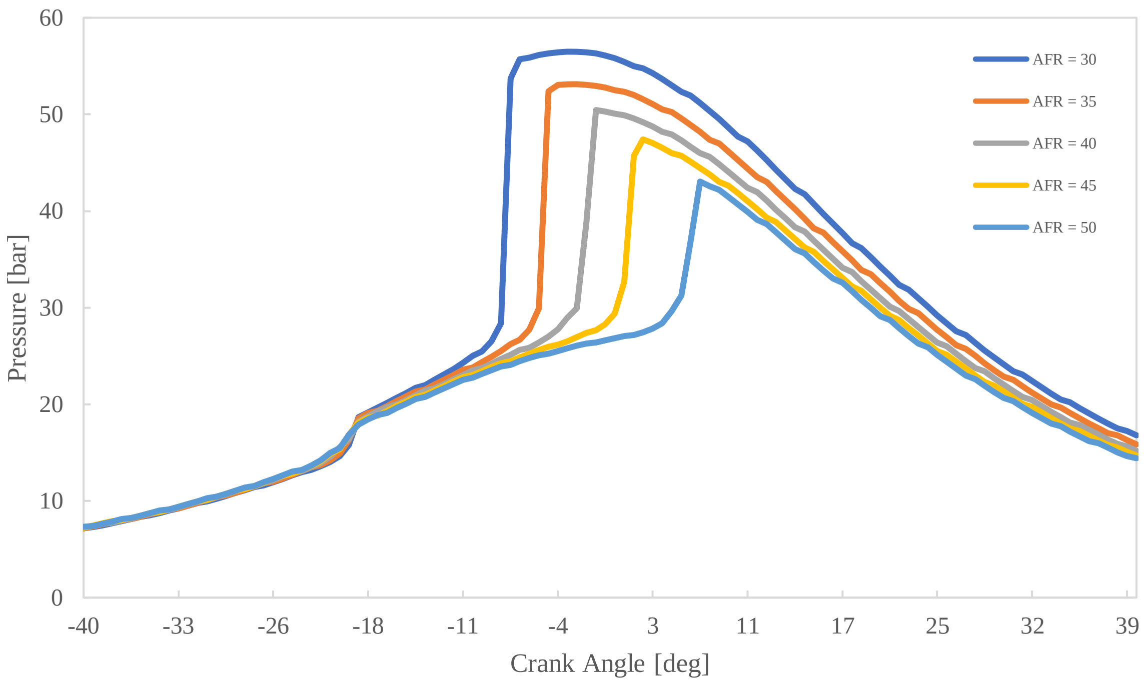

Figure 2. Effects of AFR on in-cylinder pressure

As mentioned previously, the use of n-heptane in HCCI engine tends to produce a two-stage heat release region namely the Low Temperature Heat Release (LTHR) and high temperature heat release (HTHR). Figure 3 shows that the simulation result is able to provide both LTHR and HTHR phenomena which are natural characteristics of HCCI combustion fuelled with n-heptane or diesel. The result shows that as the AFR increases, the phasing of LTHR is slightly advanced, while that of HTHR is significantly retarded. The retarded HTHR leads to the delay in the auto-ignition. This is because the molecule of hydrocarbon mixes poorly with oxygen at leaner mixtures (higher AFR). As a result, as the heat release rate of the HTHR decreases, the cumulative heat release rate also reduces. This finding shows that varying the value of AFR has the potential to control the heat release rate of HCCI combustion thus preventing the tendency of both misfire and knocking.

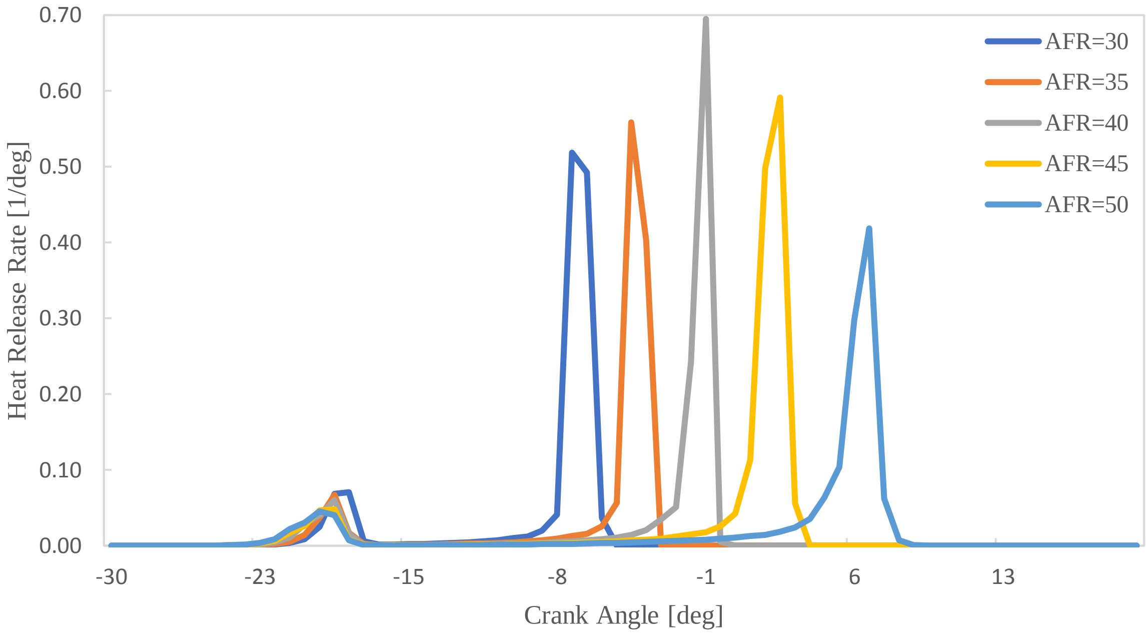

Figure 3. Effects of AFR on heat release rate

3.2. Effect of compression ratio (CR)

Another important engine parameter that is normally used to control HCCI combustion phasing is compression ratio (CR). Figure 4 shows the effect of various compression ratios on HCCI in-cylinder pressure. The value of CR was varied between 10 and 16 for a constant intake air temperature (325 K), pressure (1 bar), AFR (45), EGR (20%) and engine speed (1000 rpm).

Theoretically, increased CR will raise the peak in-cylinder pressure and advance the combustion process, resulted from the increase of compression temperatures and pressures. Figure 4 shows that the in-cylinder pressure increases significantly with the increase of CR. However, the peak pressure of all compression ratios has relatively the same crank angle position (around -5 before top dead centre) except for CR of 10. The auto-ignition of high CR is also well advanced in the crank angle position compared to that of lower CR. The reason why the CR of 10 gives the lowest peak pressure and the most retarded combustion phasing is caused by the poor oxidation of n-heptane at low compression ratio. With low CR, the temperature and pressure are not sufficient enough to ignite the fuel.

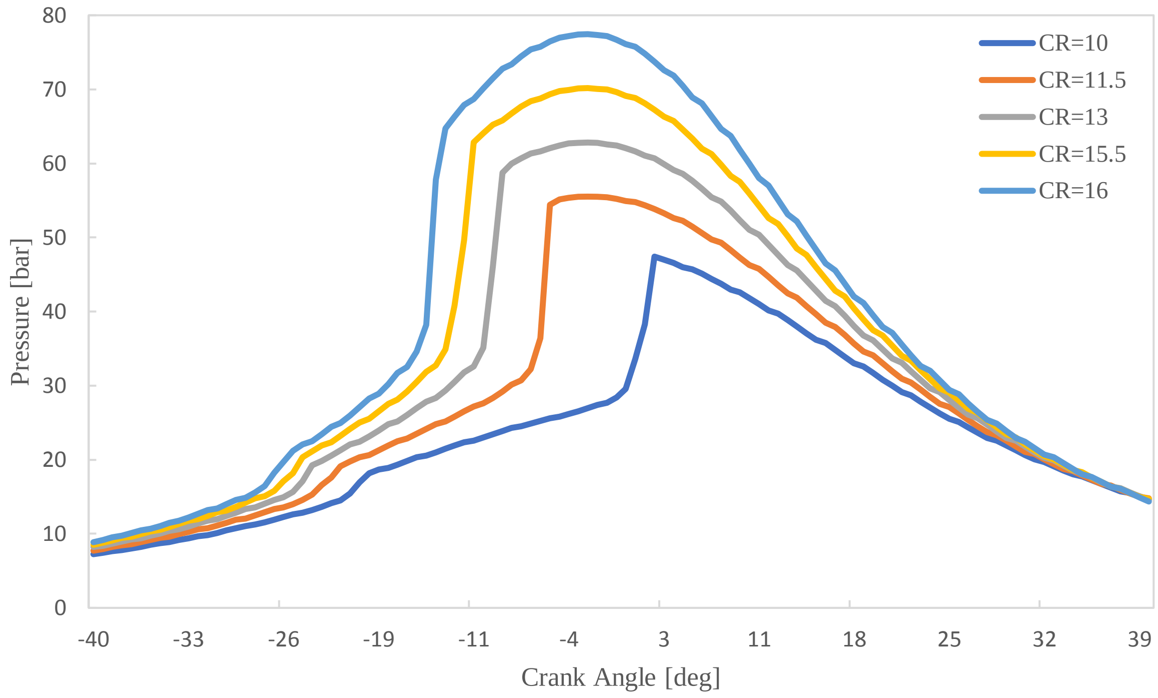

Figure 4. Effects of CR on in-cylinder pressure

Figure 5 shows the effect of various CR on HCCI heat release rate. Heat release indicates the start of the chemical reactions and the release of massive energy that will increase the in-cylinder temperature and pressure. It is shown in the figure that the higher the CR is, the more advance the heat release is. One of the main concern of using diesel fuel or n-heptane in HCCI engine is its low volatility characteristic which can cause problem in its fuel evaporation process. In some cases, wall wetting is unavoidable thus causing the incomplete combustion and increasing both unburned hydrocarbons and CO emissions. Results from Figure 5 indicate that by varying the CR, the heat release can be advanced or retarded. Therefore, changing the value of CR can be a useful strategy to control the heat release rate of HCCI engine. In addition to that, varying CR can also improve the evaporation process of low volatile fuel such as diesel and n-heptane.

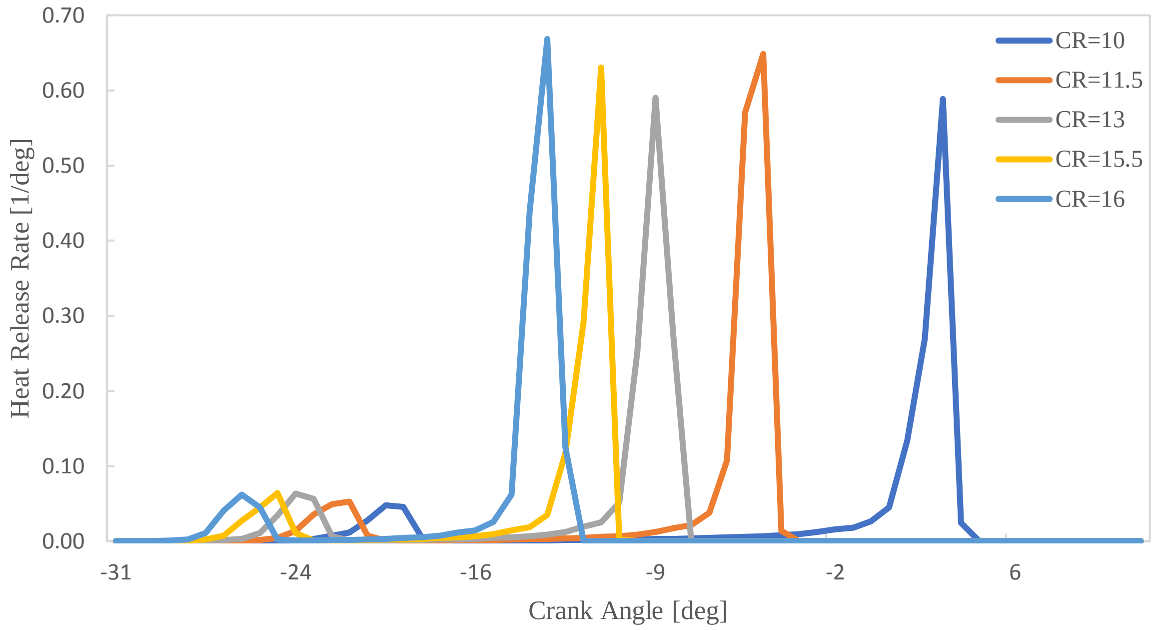

Figure 5. Effects of CR on heat release rate

3.3. Effect of intake air temperature

To control the HCCI combustion, heating the intake air temperature is often used as an effective way to control the combustion phasing. Figure 6 shows the effect of intake air temperature on HCCI in-cylinder pressure. The value of the T_{in} was varied between 300 and 360 K for a constant ambient pressure (1 bar), AFR (45), CR (10), EGR (20%) and engine speed (1000 rpm).

Figure 6 shows that as the intake air temperature increases, the auto-ignition timing advances significantly. Due to the advanced of auto-ignition timing, the pressure rise rates will increase thus resulting in rapid heat release rate. In reality, a preheating device is often used to heat the intake air. However, it is important to note that as the hot intake air enters the combustion chamber, it will mix with the fuel and is compressed during the compression stroke. This will eventually increase the charge temperature to the auto-ignition temperature of n-heptane. As a result, too early auto-ignition may occur and cause knocking. Therefore, the range of intake air temperature value has to be considered carefully. Results from Figure 6 indicate that varying the intake air temperature is a practical method to achieve the HCCI combustion using n-heptane fuel.

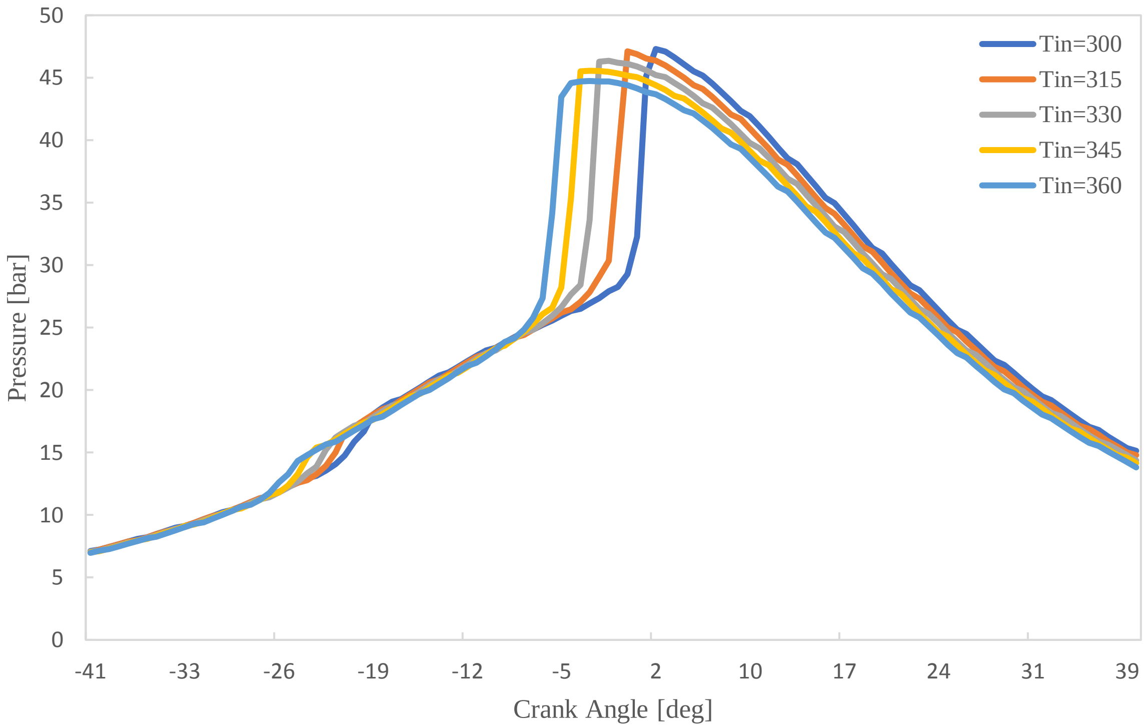

Figure 6. Effects of intake air temperature on in-cylinder pressure

Figure 7 shows the effect of various intake air temperature on HCCI heat release. The figure reveals that as the intake air temperature increases, both the LTHR and HTHR are more advanced. Consequently, knocking occurs as the peak of heat release rate is observed before TDC thereby deteriorating the HCCI combustion. As previously explained, the use of n-heptane in HCCI engine is known to produce LTHR that will increase the in-cylinder temperature [25]. In the low-temperature phase, the most important reactions of key chemical components occur i.e. $C_7H_{15}O_2$=$C_7H_{14}OOH$. This reaction will retard the process of low-temperature oxidation and cause the negative temperature coefficient (NTC) phase. Furthermore, Figure 7 also shows that a minor change in the intake air temperature will result in a major change in the heat release rate of HCCI engine. Therefore, changing the intake air temperature can play a significant role in controlling the HCCI combustion phasing.

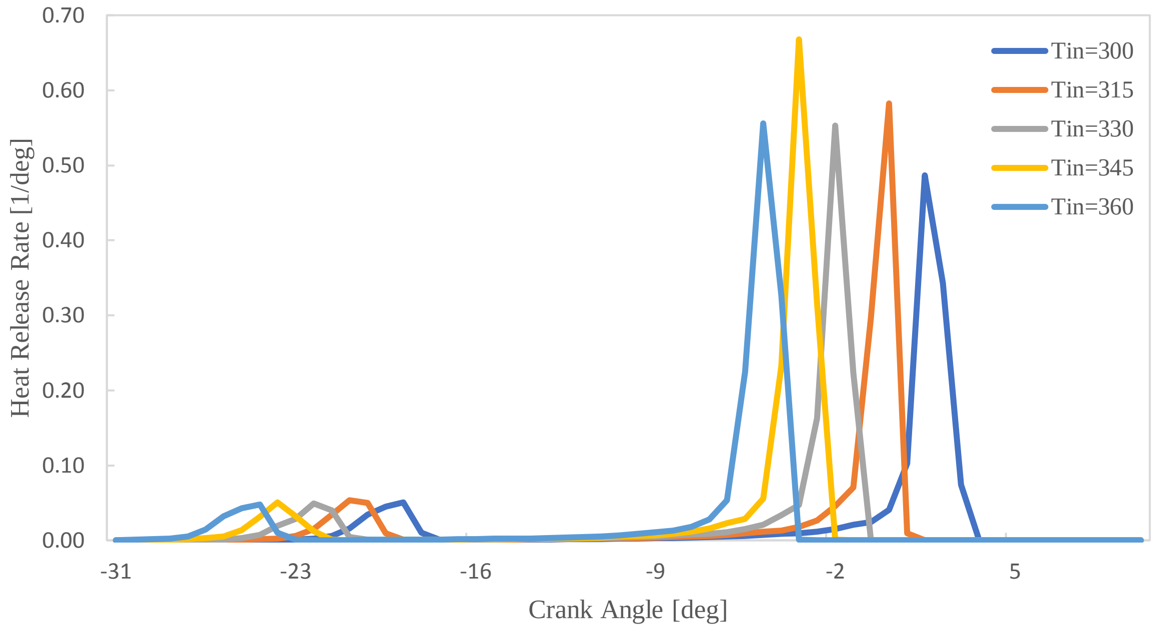

Figure 7. Effects of intake air temperature on heat release rate

4. Conclusions

HCCI fuelled with n-heptane is known to have narrow operating ranges. Its start of combustion is also difficult to regulate due to the absence of direct control mechanism. Varying a number of engine parameters can be an effective way to control its combustion phasing. A single-zone model was established to evaluate the HCCI combustion fuelled with n-heptane for different AFR, CR and intake air temperatures. The main conclusions can be summarised as follows:

- The fast and low cost of computational single-zone model was able to capture the two-stage kinetic combustion of HCCI engine namely the Low Temperature Heat Release (LTHR) and the High Temperature Heat Release (HTHR) regions.
- Decreasing the value of AFR was found to increase the pressure and temperature of combustion due to its rich mixtures composition. As the pressure and temperature increased during the compression stroke, the oxidation of n-heptane also improved thus advancing the auto-ignition timing. As a result, the pressure-rise rates increased thus causing rapid heat release rate that was prone to knock problem.
- The increase of CR and intake air temperature resulted in the increase of pressure and temperature combustion. During the compression stroke, the reactions of key chemical components depended on the in-cylinder pressure and temperature. Therefore, higher compression ratio and inlet air temperature would advance the start combustion of HCCI engine.
- Minor changes in the value of AFR, CR and intake air temperature led to significant changes in the combustion phasing. This finding indicates that both knocking and misfire can be effectively avoided if critical engine parameters are set properly. Moreover, the start of HCCI combustion can also be controlled by varying the AFR, CR or inlet air temperature.

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References

[1] Bahri B, Abdul A, Shahbakhti M, Farid M and Said M 2013 Understanding and detecting misfire in an HCCI engine fuelled with ethanol *Appl. Energy* **108** 24–33

[2] Hairuddin A A, Yusaf T and Wandel A P 2014 A review of hydrogen and natural gas addition in diesel HCCI engines *Renew. Sustain. Energy Rev.* **32** 739–61

[3] Sharma P and Dhar A 2016 Development of chemical kinetics based hydrogen HCCI combustion model for parametric investigation *Int. J. Hydrogen Energy* **41** 6148–54

[4] Hasan M M, Rahman M M, Kadirgama K and Ramasamy D 2018 Numerical study of engine parameters on combustion and performance characteristics in an n -heptane fueled HCCI engine *Appl. Therm. Eng.* **128** 1464–75

[5] Hasan M M, Rahman M M and Kadirgama K 2014 A Review on homogeneous charge compression ignition engine performance using biodiesel–diesel blend as a fuel *Int. J. Autom. Mech. Eng.* **11** 1–5

[6] Jafarmadar S, Nemati P and Khodaie R 2015 Multidimensional modeling of the effect of Exhaust Gas Recirculation (EGR) on exergy terms in an HCCI engine fueled with a mixture of natural gas and diesel *Energy Convers. Manag.* **105** 498–508

[7] Rezaei J, Shahbakhti M, Bahri B and Abdul A 2015 Performance prediction of HCCI engines with oxygenated fuels using artificial neural networks *Appl. Energy* **138** 460–73

[8] He B, Yuan J, Liu M and Zhao H 2014 Combustion and emission characteristics of a n-butanol HCCI engine *Fuel* **115** 758–64

[9] Wang Z, Liu H, Ma X, Wang J, Shuai S and Reitz R D 2016 Homogeneous charge compression ignition (HCCI) combustion of polyoxymethylene dimethyl ethers (PODE) *Fuel* **183** 206–13

[10] Tanaka S, Ayala F, Keck J C and Heywood J B 2003 Two-stage ignition in HCCI combustion and HCCI control by fuels and additives *Combust. Flame* **132** 219–39

[11] Zhang Z, Xie Q, Liang J and Li G 2017 Numerical study of combustion characteristics of a natural gas HCCI engine with closed loop exhaust-gas fuel reforming *Appl. Therm. Eng.* **119** 430–7

[12] Putrasari Y, Jamsran N and Lim O 2017 An investigation on the DME HCCI auto-ignition under EGR and boosted operation *Fuel* **200** 447–57

[13] Zhang S, Xu Z, Lee T, Lin Y, Wu W and Lee C-F 2016 A semi-detailed chemical kinetic mechanism of acetone-butanol-ethanol (ABE) and diesel blends for combustion simulations *SAE Int. J. Engines* **9** 2016-01–0583

[14] Li G, Zhang C and Zhou J 2017 Study on the knock tendency and cyclical variations of a HCCI engine fueled with n -butanol / n -heptane blends *Energy Convers. Manag.* **133** 548–57

[15] Hairuddin A A, Yusaf T and Wandel A P 2016 Single-zone zero-dimensional model study for diesel-fuelled homogeneous charge compression ignition (HCCI) engines using Cantera **13** 3309–28

[16] Broekaert S, De Cuyper T, De Paepe M and Verhelst S 2017 Evaluation of empirical heat transfer models for HCCI combustion in a CFR engine *Appl. Energy* **205** 1141–50

[17] Shahsavan M and Mack J H 2018 Numerical study of a boosted HCCI engine fueled with n-butanol and isobutanol *Energy Convers. Manag.* **157** 28–40

[18] Desantes J M, López J J, García-Oliver J M and López-Pintor D 2017 A phenomenological explanation of the auto-ignition propagation under HCCI conditions *Fuel* **206** 43–57
[19] Komninos N P 2009 Modeling HCCI combustion: Modification of a multi-zone model and comparison to experimental results at varying boost pressure *Appl. Energy* **86** 2141–51
[20] Bissoli M, Cuoci A, Frassoldati A, Faravelli T, Ranzi E, Errico G D, Milano P, Contino F and Brussel V U Detailed kinetic analysis of HCCI combustion using a new multi-zone model and CFD simulations *SAE Int. J. Engines* **2013-24-00**
[21] Bissoli M, Frassoldati A, Cuoci A, Ranzi E, Mehl M and Faravelli T 2016 A new predictive multi-zone model for HCCI engine combustion *Appl. Energy* **178** 826–43
[22] Nazoktabar M, Jazayeri S A, Arshtabar K and Ganji D D 2018 Developing a multi-zone model for a HCCI engine to obtain optimal conditions using genetic algorithm *Energy Convers. Manag.* **157** 49–58
[23] Fathi M, Jahanian O, Ganji D D, Wang S and Somers B 2017 Stand-alone single- and multi-zone modeling of direct injection homogeneous charge compression ignition (DI-HCCI) combustion engines *Appl. Therm. Eng.* **125** 1181–90
[24] Fiveland S B and Assanis D N A four-stroke homogeneous charge compression ignition engine simulation for combustion and performance studies *SAE Pap.* **2000-1**–**3**
[25] Kozarac D, Taritas I, Vuilleumier D, Saxena S and Dibble R W 2016 Experimental and numerical analysis of the performance and exhaust gas emissions of a biogas / n-heptane fueled HCCI engine *Energy* **115** 180–93