Predictive simulation of single cylinder n-butanol HCCI engine

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Abstract. Homogeneous Charge Compression Ignition (HCCI) is a commonly research new combustion mode due to its advantages over conventional combustion in internal combustion engine such as higher thermal efficiency as well as lower particulate matter (PM) and nitrogen oxides (NOx) emission. However, combustion phasing control difficulty is the main challenge in order to achieve this HCCI combustion due to the absence of direct auto-ignition control. The aim of this study is to investigate the effects of engine load conditions, intake charge temperature and exhaust gas recirculation (EGR) rate numerically on the combustion characteristics of HCCI engine in a single-cylinder and four-stroke engine fuelled with n-butanol. Predictive one-dimensional engine cycle simulation with single-zone model is employed in this study. A chemical kinetic mechanism of n-butanol is used to in this model to capture the chemical reaction process during the combustion. It was found that these parameters play important roles towards the combustion phasing of the HCCI engine as well as the in-cylinder pressure. This HCCI model is able to predict the trend of the combustion characteristics comprehensively with the variation of these critical parameters resulting in a good agreement with previous HCCI studies.

1. Introduction

Homogeneous charge compression ignition combustion has gained interests due to its advantages over conventional diesel and petrol engines. Higher efficiency over spark ignition (SI) engine and lower emission of NOx and soot compared to compression ignition (CI) engine are the main advantages of this HCCI engine [1]. HCCI combustion also can be operated using a wide variety of fuels, fuel blends and alternatives fuels [2]. This combustion mode uses lean homogeneous mixture and air-fuel mixture auto-ignition process occurs without direct mechanism control. However, due to the working principle of this HCCI engine, the major challenge is to control the combustion phasing or the start of the combustion. Many researchers previously employed several strategies to control the HCCI combustion such as controlling the intake charge temperature [3], [4], exhaust gas recirculation [5], [6], varying the air-fuel ratio [7], [8] and many more.

Butanol was proven to be able to fuel the HCCI engine in numerous studies previously [3], [9], [10]. Out of the different isomers of butanol which are n-butanol,isobutanol,tert-butanol and sec-butanol, n-butanol had been investigated the most in engine studies [3]. Compared to other alcohol fuels, butanol has several advantages in terms of energy content and suitability to be blended with diesel or gasoline [11], [12].

A few approaches can be used in modelling HCCI combustion including single-zone model and multi-zone model [13]. In single zone model, combustion chamber is assumed to have uniform temperature, pressure and composition throughout its internal space, thus, computation time is reduced. Besides, it is reported that this model presents ideal HCCI combustion [14]. However, it cannot accurately predict the heat release rate, combustion duration and the rate of pressure change [13]. Veza et al. [15] investigated combustion characteristics of n-heptane HCCI engine using single zone model by varying the compression ratio (CR), air-fuel ratio (AFR) and intake temperature. It is found that single-zone model can predicts the two-stage heat release rate process in HCCI combustion. Also, increasing the intake temperature, CR and decreasing the AFR resulted in advanced combustion phasing. On the other hand, Shahsavan and Mack [3] employed single-zone model using four different kinetic mechanisms of n-butanol to study the HCCI combustion with varying intake pressure, equivalence ratio and intake temperature. It was clearly reported that increasing intake temperature advanced the combustion timing in all operating conditions in which the trends were similar to experimental data.

The aim of the present study is to investigate the effects of three parameters including engine loads, intake charge temperature and EGR rate on the combustion timing of n-butanol HCCI engne using a developed engine cycle model with a reduced kinetic mechanism. Intake charge temperature, EGR rate and engine load conditions are believed to have significant impact on the behaviour of HCCI combustion for controlling the combustion phasing. Proper combustion phasing control is essential in HCCI engine due to the lack of direct control of combustion phasing in this engine. This study also took the advantages of low cost and less time consuming of single-zone computational model to predict the combustion characteristics of HCCI engine fuelled with n-butanol.

2. Methodology

Figure 1 illustrate the one-dimensional engine cycle model used in this study from intake system to the exhaust system. The specification of engine cylinder geometry follows four-stroke and single cylinder Yanmar L70N diesel engine model with CR = 20:1, bore = 78 mm, stroke = 67 mm and connecting rod length = 102 mm. In this model, Woschni GT heat transfer model was used for in-cylinder heat transfer prediction. This model is a modified classical Woschni heat transfer model where the heat transfer is increased by inflow velocities through the intake valves and also by backflow through the exhaust valves during the period of valves opening. The AFR were set based on the corresponding BMEP values to maintain the engine speed at 2000 rpm while the fuel delivery rate was fixed at 7 g/s. Different load conditions required different amount of fuel and air for the engine to run in a constant speed mode. Table 1 shows the simulation matrix of the present study.

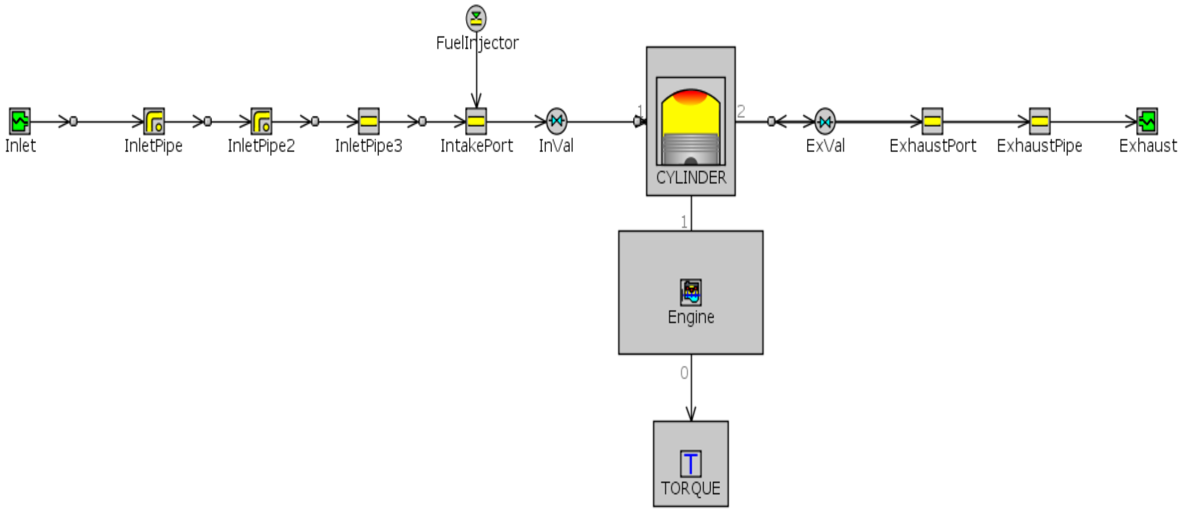

Figure 1. One-dimensional engine cycle model

Table 1. Simulation Matrix

BMEP (bar)	EGR Rate (%)	Intake Charge Temperature (K)	Intake Pressure (bar)	Speed (rpm)	AFR
1.18	0	300	1	2000	39
1.96	0 – 50	300 - 360	1	2000	35
2.75	0	300	1	2000	29
3.53	0	300	1	2000	23

Due to the absence of direct control mechanism for the auto-ignition process, several strategies were commonly employed to achieve HCCI combustion including controlling the intake charge temperature and EGR rate. Thus, these parameters were varied at constant engine speed, load condition and AFR to investigate its effects toward the combustion phasing of HCCI engine. A reduced mechanism of n-butanol by Wang et al. [1] was used in order to simulate the chemical kinetics of HCCI combustion with single zone model approach.

3. Results and discussion

3.1. Effects of engine load conditions

Engine load condition is one of the critical engine parameters which have great influence on the combustion characteristics. As stated previously, for each engine load conditions, different AFR is required to maintain the engine at constant speed. It is because the amount of energy required to rotate the shaft differs for every load. Higher engine load requires greater amount of energy from richer mixture (lower AFR) to ensure the engine speed maintains at the desired value and vice versa. Figure 2 shows the engine cylinder pressure versus crank angle at different brake mean effective pressure (BMEP) values at 2000 rpm engine speed and 300 K intake temperature. It is clearly shown that higher BMEP resulted in higher cylinder pressure. This is due to the combustion of richer mixture for higher load conditions that gives higher power output. Besides, the position of the peak pressure is seen to be more advanced for higher loads indicating faster combustion rate. It is reported that HCCI combustion has low operating region which is at low load condition, misfire may occurs causing combustion instabilities and at high load condition, knocking may occurs causing damage to the engine [2]. Therefore, engine load condition can be a control factor in HCCI engine.

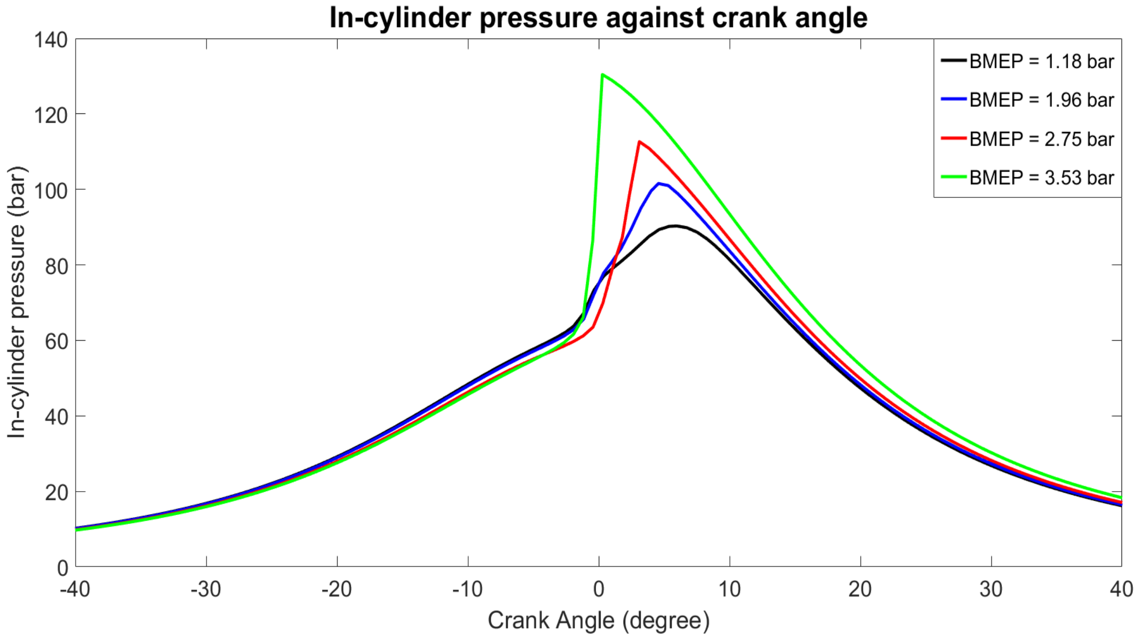

Figure 2. In-cylinder pressure against crank angle at different BMEPs with 2000 rpm engine speed and 300 K intake charge temperature.

3.2. Effects of EGR rate

One of the most common method to control HCCI combustion is by applying EGR. EGR can be categorised into two which are internal EGR and external EGR [1]. EGR influences HCCI combustion by several ways including diluting the intake charge and lowering the combustion temperature [6]. Figure 3(a) shows the cylinder pressure results with different EGR rate at 2000 rpm engine speed, 300 K intake temperature and 1.96 bar BMEP. As we can see, the cylinder pressure differs for each applied EGR rate with highest EGR rate resulted in the lowest cylinder pressure. This is due to the fact that higher EGR rate provides higher dilution to the intake charge and reduces the availability of fresh air containing oxygen for combustion [6]. Thus, this explains the lower energy output for higher EGR rate cases.

Besides, the effects of EGR can also be seen on the combustion phasing of HCCI engine. Figure 3(b) shows the result of combustion timing or the timing of which the mixture is 50% burned (CA50) at constant speed, intake temperature and load condition. Higher EGR rate resulted in later CA50 timing compared to lower EGR rate. This is because the combustion rate is slower for higher EGR rate case due to diluted intake charge that slowing down the reaction. Recirculated exhaust gas also acts as the heat energy absorber by the carbon dioxide (CO2) gas and water vapor (H2O) that increase the specific heat capacity of the mixture resulting in lower combustion temperature [1]. Therefore, controlling the amount of EGR needs to properly be done to ensure the combustion phasing is optimum at desired engine operating conditions.

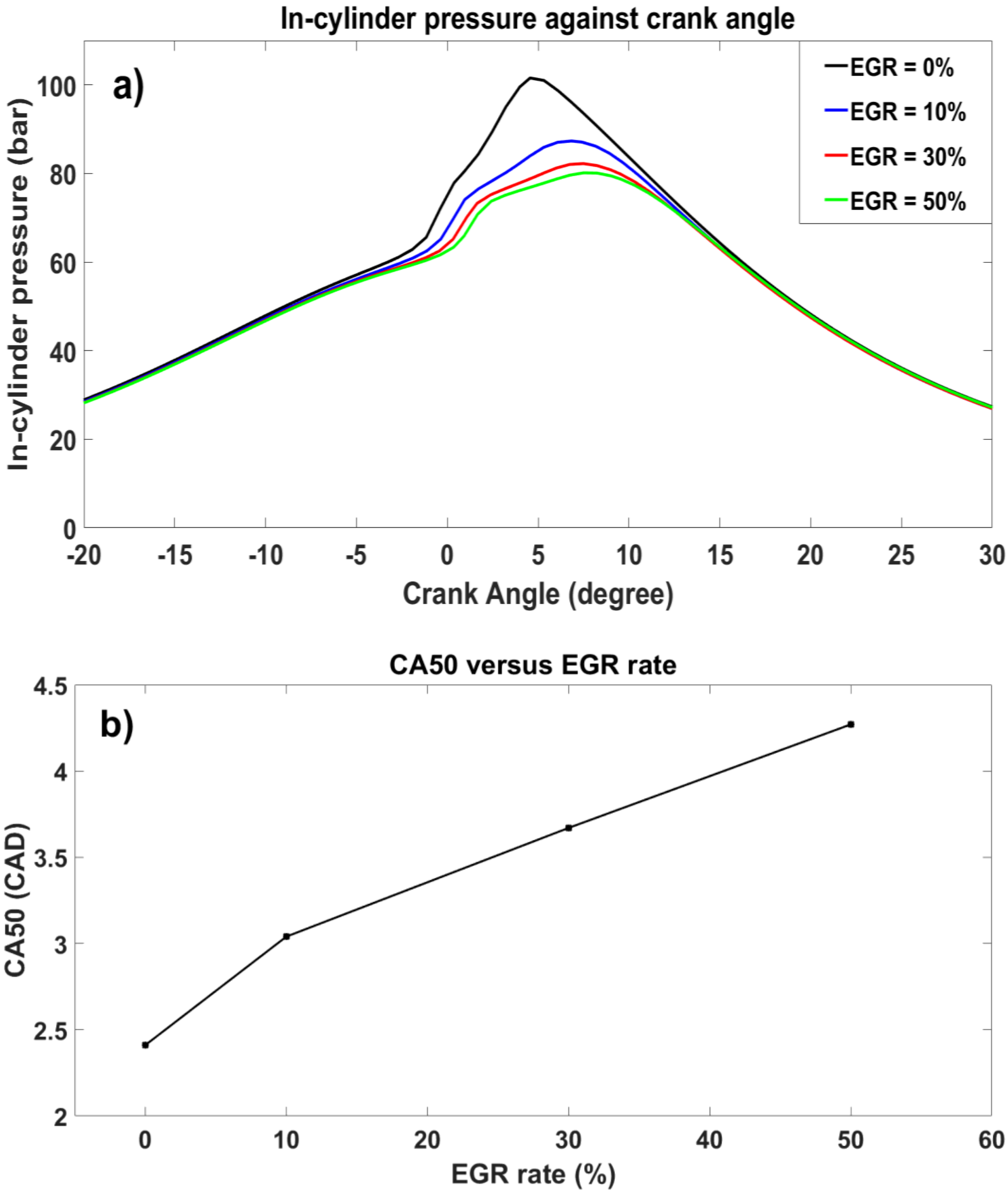

Figure 3. a) In-cylinder pressure against crank angle at different EGR rate **b)** CA50 versus EGR rate with 2000 rpm engine speed, 300 K intake charge temperature and 1.96 bar BMEP.

3.3. Effects of Intake Temperature

Controlling intake temperature is the most common strategy to control the combustion phasing of HCCI engine because it is effective to increase the rate of reaction of the mixture. Problems associated with HCCI engine such as cold start problem and auto-ignition difficulty can be solved by appropriate intake temperature raised. Figure 4 shows the effects of intake temperature on the cylinder pressure and CA50 at 1.96 bar BMEP, 300 K temperature and 2000 rpm engine speed. It can be observed that increasing the intake temperature resulted in lower cylinder pressure. This trend is also observed in previous HCCI studies using similar single-zone model [15], [18]. This is may due to the decreases of volumetric efficiency of mixture that entering the cylinder with reduced density.

Besides, CA50 affected significantly with the variation of intake temperature. Higher intake temperature causes the combustion to be advanced. This is because higher intake temperature increases the reaction rate of mixture during the compression stroke and results in earlier auto-ignition. As mentioned earlier, HCCI combustion is influenced by the chemical kinetics which is greatly affected by temperature. Therefore, increasing intake temperature will increases the heat release rate of mixture and reduces the time for the ignitable mixture to reach its auto-ignition temperature. However, this parameter needs to be properly controlled because too advanced combustion will give adverse effects toward the engine performance. Too high intake temperature will cause rapid pressure rise rate leading to knocking while too low intake temperature will not be sufficient to achieve HCCI combustion.

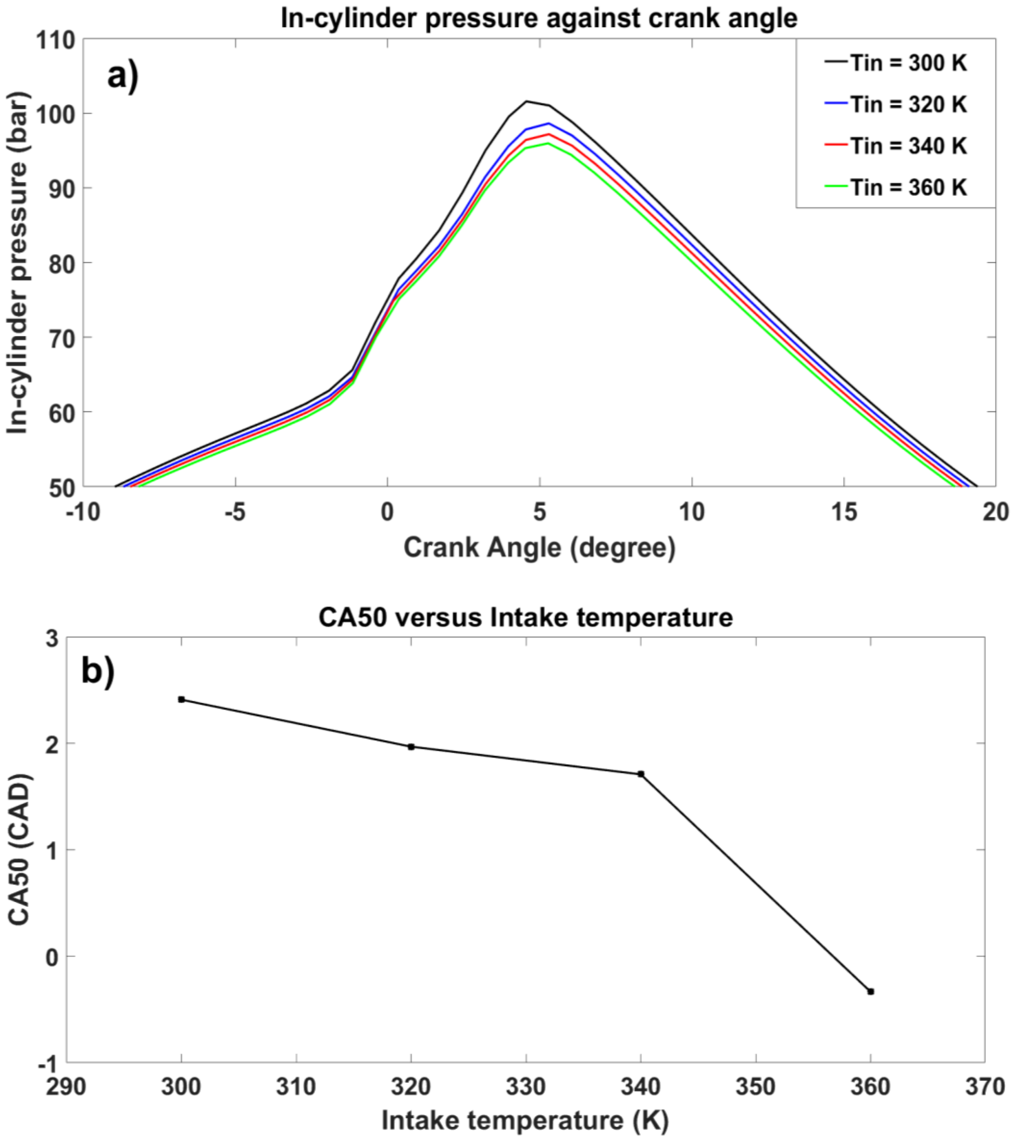

Figure 4. a) In-cylinder pressure against crank angle at different intake temperature **b)** CA50 versus intake temperature with 2000 rpm engine speed, 300 K intake charge temperature and 1.96 bar BMEP.

4. Conclusion

Narrow operating range of HCCI engine makes it difficult to control its combustion at desired engine operating conditions. Due to the absence of direct control mechanism for the auto-ignition process in HCCI engine, several strategies need to be applied to control its combustion phasing. This study investigates three parameters that have significant impact on HCCI engine fuelled with n-butanol including engine load condition, intake temperature and EGR rate. Increasing engine loads increases the cylinder pressure, advances the combustion phasing and requires lower AFR to operate in constant speed mode. Moreover, more retarded combustion is observed in higher EGR rate due to dilution effects that reduces the rate of reaction. Finally, opposite to the effects of EGR rate on combustion characteristics of HCCI engine, increasing intake temperature advances the combustion of HCCI engine due to increased reaction rate and need to be carefully controlled to avoid knocking. The observed results show similar trends to previous HCCI studies. This model can be used to predict certain required engine operating conditions for experimental HCCI study. It reduces the time and cost of experiment to select the best required operating conditions of n-butanol HCCI engine.

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