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The Combustion Behavior Analysis of Dual Fuel HCCI using the Shell Model

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Abstract: Homogeneous Charge Compression Ignition (HCCI) engine has become a potential power unit to satisfy the stricter emission regulations and obtain higher thermal efficiency values. However, main issues are the uncontrollable combustion of HCCI, which is unfavorable for engine application. Dual fuel application in HCCI is applied to overcome the difficulty in combustion control. There are some research has been done, but the research that focused on the combustion behavior of the dual fuel has not yet been investigated. Current research objective is to simulate and analyze the affecting parameters and the behavior of the dual-fuel HCCI combustion. The simulation was done on constant volume chamber using the SHELL autoignition model. It is shown that initial temperature has the major effect to the combustion delay of dual fuel. Higher initial temperature will shorten the combustion delay. Furthermore, the existence of fuel with higher octane number suppressing the reaction and delay the combustion.

Key words: HCCI, dual-fuel, combustion, simulation

INTRODUCTION

HCCI is a combustion system that combined main characteristics of the establish IC engine, spark ignition (SI) and compression ignition (CI) engine. HCCI used auto-ignition to ignite a homogeneous mixture of fuel and air in order to get higher thermal efficiency and lower exhaust emission compared to its predecessor. Furthermore, HCCI able to reduce the fuel consumption due to it is operate in a very lean condition.

The HCCI concept was originally introduced by Onishi *et al.* (1979) to improve the combustion stability on two stroke gasoline engines. They found that there are significant improvement in fuel economy and reduce in exhaust emissions. Furthermore, Noguchi *et al.* (1979) performed optical investigations on this system. They found that there was no discernable flame front during the combustion process. Najt and Foster extended the work to four stroke spark ignition engine and they concluded that the HCCI combustion was governed by low temperature chemistry (<1000 K) while the bulk heat release controlled by high temperature chemistry (>1000 K).

Earlier works in HCCI combustion have open new possibilities of combustion system. However, there are some drawbacks of HCCI employment on the real engine. Among all of the drawback, limited operating range become the main focus for the next development of HCCI combustion system. This limited operating range is due to

the difficulties of controlling the auto-ignition process that contains many affecting parameter.

The combustion of homogeneous charge compression ignition engine (HCCI): Controlling the auto-ignition on HCCI combustion requires better understanding on the auto-ignition process especially on the factors that affecting the fuels to be auto ignite in the HCCI combustion system. The auto ignition process is mainly governed by chemical reaction occurs in the environment that provides sufficient energy to be used. The minimum energy required for the chemical reaction to starts is called activation energy and it varies for different fuels.

In the HCCI combustion system, the chemical reaction involved can be classified into four stages; Low Temperature Heat Release (LTHR) that occur after the charge temperature achieving 600 K, Intermediate Temperature Heat Release (ITHR) occurs at the 950 K and High temperature heat release (HTHR) that occurs above 1000 K (Hultrvist *et al.*, 2008) and burnout.

Furthermore, based on the governed combustion stages, the fuel characteristics can be classified into two categories: single stage ignition and two stage ignition fuels. The combustion of single stage ignition fuels can be identified by one peak heat release in the Heat Release Rate (HRR) graph. The chemical reaction of these fuels only occurs at the temperature of more than 950 K which is at the HTHR region. This single stage ignition behavior can be seen in the application of gasoline and natural gas

fuel. While the two stage ignition fuels, the HRR graph shows two peak values which is at LTHR and HTHR region. The heat release drop after LTHR region occur due to the negative temperature coefficient zone occurs. In this ITHR zone, the reaction rate will be slowing down near to zero even though the temperature keeps increasing. This two stage ignition behavior commonly associated with diesel fuel and on the lighter fuel such as naphtha and JP8 (Yao *et al.*, 2009).

Current research on the affecting parameters of HCCI combustion system: Hwang *et al.* (2008) investigated the HCCI combustion phase for single and two stage ignition fuels. The experiment was done using optically accessible engine with 981 cc displacement volume, 18:1 compression ratio, at 1200 RPM. The engine temperature was maintained 100°C for the whole experiment and fuel supply was done using port and direct injection method. The fuel used were iso-octane for the single stage ignition and PRF80 for the two-stage ignition. It was found that the single stage ignition fuel has three distinct stage of combustion, ITHR, HTHR and burnout. Iso-octane shows slow temperature rise during ITHR phase and the chemiluminescence images showed weak uniform emission that mainly consists of formaldehyde. In HTHR, a rapid temperature rise rate was occurring during this phase. Hotter temperature region will showed very bright chemiluminescence indicate the CO continuum occurred. The CO continuum will occur if only the temperature of combustion had reached over 1170 K and this also shows that there are strong correlation between chemiluminescence and heat release rate in the combustion process.

Combustion phase using two-stage ignition fuel as stated by Hwang *et al.* (2008) has 4 stages, LTHR, ITHR, HTHR and burnout. From the ITHR to burnout stage, the combustion of PRF80 was similar to that iso-octane. However, for two-stage ignition fuel, LTHR or cool flame phenomenon is occur. There will be notified heat released detected during the combustion temperature 760-880 K and chemiluminescence spectrum showed weak formaldehyde emission.

Other researcher Lu *et al.* (2005) had similar result of the two stage ignition fuel. Lu *et al.* (2005) was using single cylinder originally diesel engine. The compression ratio used is 18.5:1 and the fueling system was using direct injection method with 5.5 MPa injection pressure. The fuel being tested was PRF fuels with octane number 0 (n-heptane), RON25, RON50, RON75 and RON90. The results showed in the first combustion phase that the octane number and equivalence ratio gives significant

impact on the combustion. The start of ignition retards, the maximum heat release rate decreases, and the pressure and temperature rise is decreasing with the increase in research octane number (RON) and decrease in equivalence ratio. While in the second phase of the combustion the combustion duration is decreasing as the increase of equivalence ratio and decrease in RON. However, the start of ignition for the second phase is linear with the first phase. Furthermore, the cycle-by-cycle variation was decreasing with the increase in equivalence ratio and cetane number.

Diverse combustion characteristics of every fuel in HCCI combustion give an opportunity to combine two or more fuels in order to control and improve the combustion process. Some of the previous research has proven that dual fuel is a mean way to control the combustion which usually employed with the combination of low octane fuel and high octane fuel. Where the objective is to achieve HCCI combustion especially in cold-start and idle load condition. This fuel combination can leads to a higher operating range of HCCI engines (Kong, 2007; Yeom *et al.*, 2007; Shudo and Yamada, 2007; Ma *et al.*, 2008; Machrafi and Cavadias, 2008).

Along with the potential of dual fuel application on HCCI engine, the combustion behavior of this fuel combination is not yet investigated. The affecting parameter such as initial temperature, the fuel composition in the mixture, and total equivalence ratio are among the parameters that proven to be affecting the autoignition process in HCCI engine. So, the current investigation will observe these parameters effect to the autoignition process in the HCCI engine.

The simulation approach will be used to investigate this behavior of dual fuel autoignition process. The Shell model will be used for the chemical kinetics calculation due to its capability to predict the knocking in the gasoline and diesel engine with acceptable accuracy. The Shell model used simplified chemical kinetics model in order to reduce time consumed for the simulation process (Sazhin *et al.*, 1999; Shazina *et al.*, 1999).

MODEL DEVELOPMENT

The Shell model consists of 8 reactions and represent 4 main stages of chemical reaction occur in the combustion process. The Shell model used a simplification method where all the radicals involved in the chemical reaction of hydrocarbon fuel as one substance and this model had reduced the reaction to only the major reaction that gives significant contribution to the reaction rate of the chemical reaction.

The four stages of chemical reactions are:

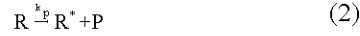
$$[RH] = \frac{[O_2] - [O_2](t=0)}{p^n} + [RH](t=0) \quad (13)$$

- Initiation:



The rate constants for every species can be defined by the following expressions:

- Propagation:



$$f_1 = A_{f1} \exp\left(\frac{-E_{f1}}{RT}\right) [O_2]^{p1} [RH]^{q1} \quad (14)$$



$$f_2 = A_{f2} \exp\left(\frac{-E_{f2}}{RT}\right) \quad (15)$$



$$f_3 = A_{f3} \exp\left(\frac{-E_{f3}}{RT}\right) [O_2]^{p3} [RH]^{q3} \quad (16)$$



- Branching:

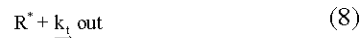


$$k_1 = A_1 \exp\left(\frac{-E_1}{RT}\right) \quad (18)$$

- Termination:



$$k_p = \left[\frac{1}{k_{p1}[O_2]} + \frac{1}{k_{p2}} + \frac{1}{k_{p3}[RH]} \right]^{-1} \quad (19)$$



where, [M] is the molar concentration of the species M. i is p1, p2, p3, q, B, and t. R is the universal gas constant (R = 1.9782 cal/mole K).

where, RH Representing fuels (C_nH_{2m}), R* representing radicals, B is the branching agent and Q is the intermediate agent. The products of the current model consist of CO₂ and HO₂ which represent a complete combustion process. The branching agent is related to the Hydroperoxide (RO₂H) at low temperature and to hydrogen peroxide (H₂O₂) at high temperature. Furthermore, the intermediate species is generalized as aldehydes (RCHO).

The parameter of p is obtained from the overall product path of:



where:

$$p = \frac{(2n+m)}{2m} \quad (21)$$

The time variation of the species concentration is described by:

$$\frac{d[R^*]}{dt} = 2(k_1[RH][O_2] + k_6[B] - k_1[RH]^2) - f_3 k_p [R^*] \quad (9)$$

$$p = \frac{n}{m} + 1 \quad (22)$$

$$\frac{d[B]}{dt} = f_1 k_p [R^*] - f_2 k_p [Q][R^*] - k_b [B] \quad (10)$$

Moreover, the time variation of the temperature changes of the chemical reaction is defined as:

$$\frac{d[Q]}{dt} = f_4 k_p [R^*] - f_2 k_p [Q][R^*] \quad (11)$$

$$\frac{dT}{dt} = \frac{1}{C_v n_{tot}} k_p q V [R^*] \quad (23)$$

$$\frac{d[O_2]}{dt} = -p k_p [R^*] \quad (12)$$

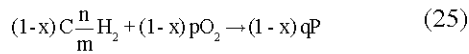
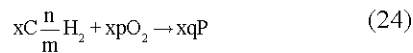
Derived from the main single fuel model, the Shell model was expanded to simulate the dual fuel autoignition process. However, due to the complicatedness of the

Table 1: Chemical reaction properties of fuels (Sazhin et al., 1999)

	90 RON	100 RON
ap1	1.00E+12	1.00E+12
ep1	0	0
ap2	1.00E+11	1.00E+11
ep2	1.50E+04	1.50E+04
ap3	1.00E+13	1.00E+13
ep3	8.50E+02	8.50E+02
aq	1.20E+12	3.96E+13
eq	3.50E+04	4.00E+04
ab	4.40E+17	6.51E+15
eb	4.50E+04	4.00E+04
at	3.00E+12	3.51E+12
et	0.00E+00	0.00E+00
af1	7.30E-04	7.30E-04
ef1	-1.50E+04	-1.50E+04
af2	1.80E+02	1.80E+02
ef2	-7.00E+03	-7.00E+03
af3	1.47E+00	2.21E+00
ef3	1.00E+04	1.00E+04
af4	1.88E+04	1.70E+04
ef4	3.00E+04	3.00E+04
x1	1.00E+00	1.00E+00
y1	0.00E+00	0.00E+00
x3	0.00E+00	0.00E+00
y3	0.00E+00	0.00E+00
x4	-1.00E+00	-1.00E+00
y4	3.50E-01	3.50E-01

gasoline fuel hydrocarbon chemical composition, the fuels were assumed as iso-octane (C₈H₁₈) with different properties of reaction rate that is shown in Table 1.

The dual fuel combustion model was made by determining the air amount required to get a complete combustion of each fuel with total lambda of the mixture is equal to 1. The fuel and air composition of the dual fuel was determined by:



The Shell model was applied to these reactions to simulate the chemical reaction that occurs in both reaction paths.

MATERIALS AND METHODS

The autoignition of the dual fuel was simulated with the effect of fuel composition, initial temperature and equivalence ratio. There are four initial temperatures applied, 250, 350, 450 and 550°C, and five equivalence ratios, 0.1, 0.3, 0.5, 0.7 and 1. Furthermore, this dual fuel autoignition model was applied to the cylindrical constant volume chamber with the total volume is 0.0002512 m³.

RESULTS AND DISCUSSION

Temperature effect: The effect of initial temperature to the combustion delay of dual fuel was simulated at the fuel composition of 10% RON90 gasoline and 90% of RON100 gasoline and is depicted in Fig. 3a-d. It was clearly seen in Fig. 1 that the temperature increment causes the combustion delay to be reduced exponentially.

While the initial temperature of 250°C shows 130 msec, the initial temperature of 550°C has 0.04 msec combustion delay time which is around 10⁴ time reduction. This rapid reduction of combustion delay time occur due to the higher initial energy provided by the temperature in order to break the fuel molecule bond.

Fuel composition effect: Three different percentage of fuel mixture was simulated in order to analyze the fuel composition effect to the combustion delay of dual fuels. 10, 50, and 90% of gasoline RON90 relative to RON100 was simulated, respectively. Figure 2 shows the fuel composition effect to the combustion delay at total equivalence ratio of the mixture is 1.

It is observed that the increment of the fuel with higher octane number causing the combustion delay time increased and the existence of higher octane fuel are

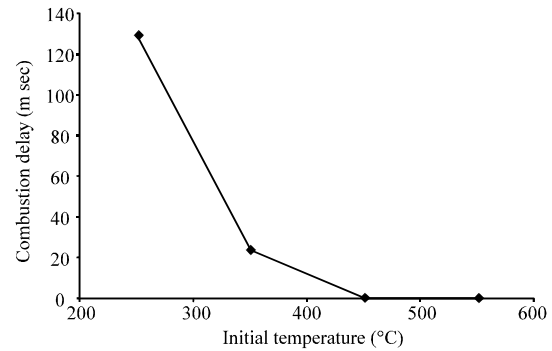


Fig. 1: Effect of initial temperature to the combustion delay of dual fuel

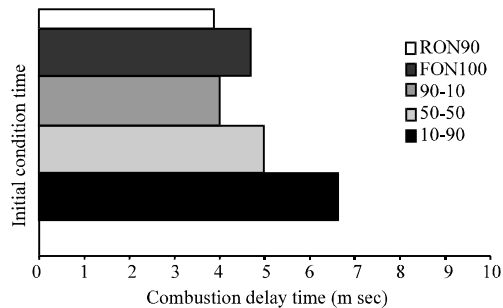


Fig. 2: The effect of fuel mixtures on the combustion delay of dual fuels at equivalence ratio of 1

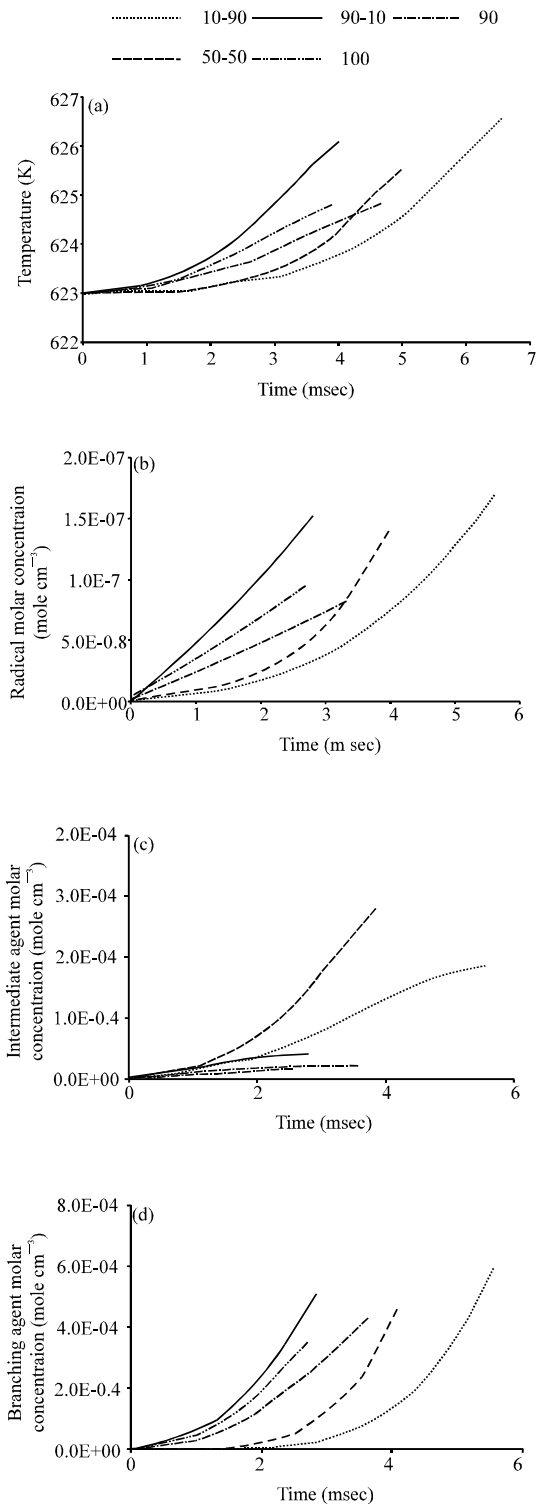


Fig. 3: Temperature and Radical, branching, intermediate concentration for dual fuel (a) Temperature (b) Radical concentration (c)Intermediate agent (d) Branching agent

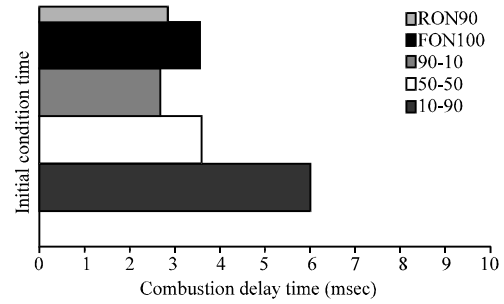


Fig. 4: The effect of fuel mixtures on the combustion delay of dual fuels at equivalence ratio of 0.1

suppressing the capabilities of the mixture to be autoignited at the same initial temperature condition. This trend is related to the agent's molar concentrations shown in Fig. 3. During the beginning of the chemical reaction, the rate of formation of intermediate agent on dual fuel combustion is faster than the formation rate of the branching agent and caused the delay of chemical chain branching. This chain branching delay is directly related to the formation of the radicals in the later process and eventually affecting the rate of temperature increase and the start of combustion.

It can be seen in the Fig. 3, the branching agent concentration is increasing as the percentage of the RON100 fuel is increased and steeply increase as the mixture temperature closing in to the autoignition temperature. The branching agent, which is consists of peroxides, is a highly flammable mixture. So, high concentration of this agent also indicates the autoignition will occur.

Figure 4 shows the combustion delay time for the fuel mixtures at equivalence ratio of 0.1. The mixtures shows the same autoignition trends as the equivalence ratio is changing. It shows that the equivalence ratio has no effect on the autoignition process itself. It can only affecting the time delay of the combustion.

However, the significant difference on the trends of the agents either its intermediate or branching to produce the radicals is observed.

The 10-90 fuel mixtures shows high concentration of intermediate agent and low branching agents during the early 3 msec after the test condition is achieved while other fuel mixture and the single fuels has high concentration of branching agents during the first 3 msec.

Furthermore, the suppressing behavior of higher octane number fuels is clearly seen in Fig. 5a-d. It shows that the increasing percentage of the fuel with higher octane number able to prolong the formation rate of the branching agent and delay the combustion. Other understanding that can be derived from these

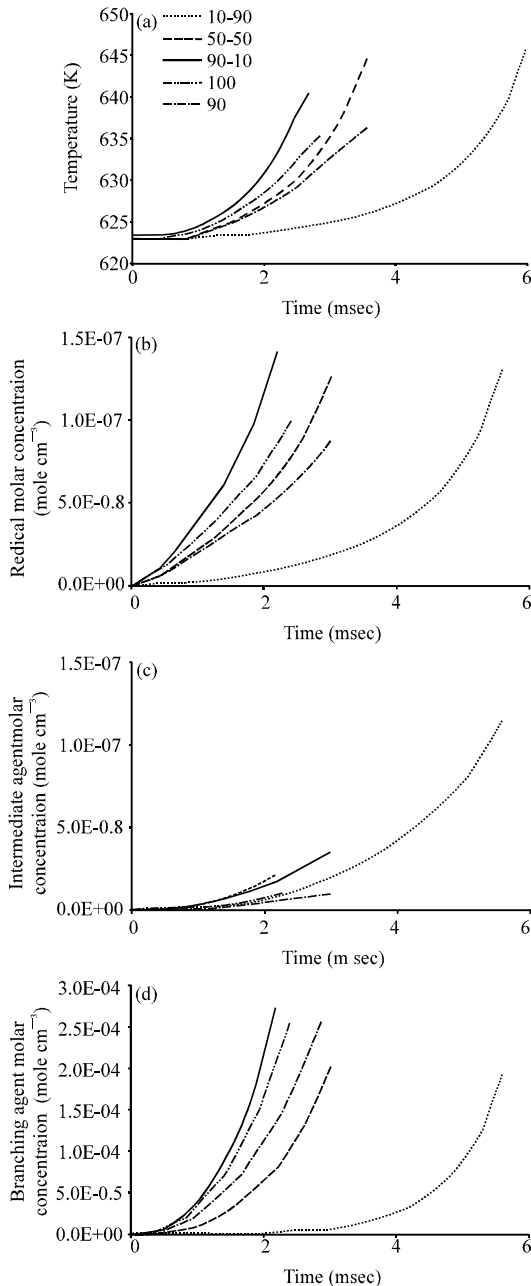


Fig. 5: Temperature and Radical branching, intermediate concentration for dual fuel; (a) Temperature (b) Branching agent (c) Intermediate (d) Radical

trends is the fuel with lower octane number highly affecting the chemical reaction during the low temperature region while the higher octane number fuel will remain steady during this region. As the temperature increase due to the early reaction with low octane number fuel, the fuel with higher octane number will starts to react and rapid rate of chemical reaction occurs.

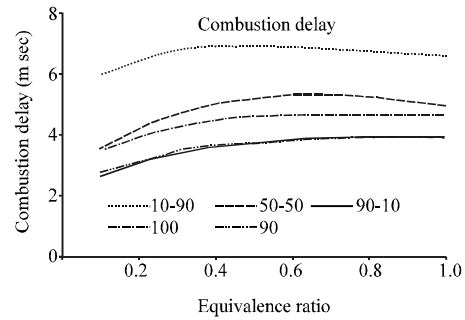


Fig. 6: The effect of equivalence ratio to the combustion delay of dual fuels

This results has the similar explanation as Hwang *et al.* (2008) where he stated that fuel with lower octane number starts to react at low temperature region and fuel with higher octane number will starts to react only at high temperature region.

Equivalence ratio effect: The effect of equivalence ratio to the combustion delay of dual fuel is depicted in Fig. 6. It shows that the combustion delay for fuel and mixtures of fuels with higher octane number has increasing trends of combustion delay as the equivalence ratio is reduced. It shows RON100 and 10-90 mixtures shows increment of combustion delay up to certain equivalence ratio the combustion delay will drop significantly.

However, the fuels and mixtures with lower octane number shows decreasing trends of combustion delay as the equivalence ratio are reduced. It shown by RON90, 90-10 mixtures, and 50-50 mixtures that the combustion delay is moderately reduced until the equivalence ratio of 0.3 the delay reduced significantly.

The steep reduction of combustion delay at the equivalence ratio between 0.1-0.3 occurs due to the high formation rate of branching agents on the beginning of the reactions as it will reduced the combustion delay of the mixture at lean condition.

CONCLUSION

The autoignition process of dual fuel in a constant volume chamber has been simulated. The effect of initial temperature, fuel mixture composition and equivalence ratio had been observed. From these data, it can be concluded that the autoignition of dual fuel are:

- Highly affected by the initial temperature due to higher energy supply to fulfill the activation energy requirement

- Affected by the fuel composition of the mixture. The composition of fuels with high and low octane number caused the chemical reaction of lower octane number fuel at low temperature is suppressed by the higher octane fuel and longer combustion delay will be occurring
- Affected by the total equivalence ratio and octane number of the mixtures. In the mixtures with high total octane number, the combustion delay is increasing as the equivalence ratio reduced. While in the mixture with low total octane number, the combustion delay is reducing as the equivalence ratio reduced

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