Single Zone Model for HCCI Engine Fueled with n-Heptane

Thanapiyawanit Bancha, and Lu Jau-Huai

***Abstract*—**In this study, we developed a model to predict the temperature and the pressure variation in an internal combustion engine operated in HCCI (Homogeneous charge compression ignition) mode. HCCI operation begins from aspirating of homogeneous charge mixture through intake valve like SI (Spark ignition) engine and the premixed charge is compressed until temperature and pressure of mixture reach autoignition point like diesel engine. Combustion phase was described by double-Wiebe function. The single zone model coupled with an double-Wiebe function were performed to simulated pressure and temperature between the period of IVC (Inlet valve close) and EVO (Exhaust valve open). Mixture gas properties were implemented using STANJAN and transfer the results to main model. The model has considered the engine geometry and enables varying in fuelling, equivalence ratio, manifold temperature and pressure. The results were compared with the experiment and showed good correlation with respect to combustion phasing, pressure rise, peak pressure and temperature. This model could be adapted and use to control start of combustion for HCCI engine.

***Keywords*—**Double-Wiebe function, HCCI, Ignition enhancer, Single zone model.

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I. Introduction

RESEARCH and development in engine performance and emission are keeping enthusiastically to meet the stick emission regulation and fighting against the driving up oil price. The ideal ICE model is well known as Otto-cycle to predict the efficiency that engine should be operated. The present commercial engines still indicate the room to develop. Regardless gasoline engine or diesel engine, they depleted a lot of limited fossil fuel even though they have shown its own advantage. Considering the type of engine; gasoline engine could operate cleaner than diesel engine, however diesel engine shows higher in thermal efficiency. These inspire the idea of hybrid among two common type of engine so far. It calls "HCCI" concept [1], [2].

To operate in HCCI mode, as the word of homogeneous charge, mixture of air/fuel is premixed around intake section and inducted through intake valve into the combustion chamber like conventional SI mode. The word "compression ignition" defines the combustion characteristics of this engine as autoignition of a usually homogenous air/fuel mixture occurs after increasing in mixture temperature and pressure in compression stroke like CI (Compression ignition) mode. Therefore changing the power output of an HCCI engine is achieved by adjusting the injection rate.

TABLE I
NOMENCLATURE

Symbol	Quantity
a	Crank radius
α	Fraction of mixture that burn in the slow combustion
B	Cylinder bore
C_v	Constant volume specific heat
E_a	Activation energy
K	Ratio of the slow burn duration to the standard burn duration
l	Connecting rod length
m	Adjustable constant
n	Polytropic coefficient
P	Pressure
Q	Heating value
R	Gas constant
T	Temperature
t	Time
V	Volume
x_b	Mass fraction burned
φ	Equivalence ratio
θ	Angle (Degree)
η_c	Combustion efficiency
SUBCRIPTS	
c	Compression
cl	Clearance
cyl	Cylinder
e	Expansion
ivc	Inlet valve close
o	Reference
soc	Start of combustion

Both SI and CI mode use spark plug and injector to control SOC (Start of combustion) respectively and result in stratified burning or flame movement from the ignited point to the surrounding. However, since there is neither spark plug nor injector in the cylinder of an HCCI engine, we need a device to control SOC precisely. Fortunately, it is well known that high temperature and pressure during compression stroke could enhance autoignition as kinetic control is the dominant factor in the initial stage of combustion. Combustion is assumed to occur everywhere thoroughly in the cylinder [1]. The sudden release of heat would cause higher temperature and pressure compared with the conventional engine [2]. However, it leads excessive PRR (Pressure rise rate), noise and harmful effect to engine as tradeoff. Therefore practical HCCI engines are always operated under extremely lean/diluted condition and the optimized equivalence ratio needs to be lower than conventional engine, ranging from 0.30 to 0.55 [5], [6].

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Intake charge temperature is an important factor to promote and control SOC. Intake air is heated and drawn into cylinder or some portion of exhaust gas is trapped or reused in order to heat next cycle mixture as called EGR (Exhaust gas recirculation). Depending on equivalence ratio, fuel and CR (Compression ratio), preheating temperature is in the range between 30 to 140°C [7].

The temperature and pressure variations during compression stroke between IVC and SOC could be modeled as a polytropic process. HCCI engine also requires high CR to achieve SOC as diesel engine does. Most engines that have been converted to HCCI mode employed diesel engine or high CR gasoline engine with at least 12:1 of compression ratio. Maiboom A., et al (2007) used diesel engine with CR of 18:1 and found that the required inlet temperature were between room temperature to 65°C. Larger CR engine could decrease the requirements of high intake charge temperature, and in some cases, ambient intake temperature could be used [8]. Increasing the CR also facilitates autoignition and expands the range of HCCI combustion mode since temperature could achieve the point of autoignition as a terminus of temperature trajectory is expanded [7], [9].

Considering the composition of mixture, the larger equivalence ratio contains more fuel portion and cause temperature increasing during compression stroke not as much as pure air. At engine with CR of 20, the highest temperature combustion is kinetic dependency, increasing in equivalence ratio of 0.2 to 1.0 at the end of compression stroke made 100 °C different of peak compression temperature. Since the large equivalence ratio imply higher heat capacity as more fraction of fuel and cause lower in the peak temperature and consequently fail in autoignition [9].

To predict the HCCI operation simply, a zero-dimensional or single zone model has been performed in this work, in accordance with [10]. The cylinder charge is assumed homogeneous in both temperature and composition. It showed ability to predict SOC and the relation between pressure and temperature in cylinder to imply heat release analyze [11]. However SOC or autoignition is an empirical model exploit "knock integral technique" and is function of cylinder temperature and pressure, equivalence ratio as well as A/F ratio. In spite of the work of [13], SOC was predicted from temperature, pressure undergo compression stroke and engines speed. Nevertheless model could not use with very late combustion timing.

In HCCI engine, there are usually large differences in effective burn rate due to temperature gradients. Peak combustion pressure predicted by single zone model always overestimated. Hence, the addition of double-Wiebe function model was accounted to separate the slower combustion that occurs in the cooler boundary region near the walls and the faster combustion in the hot core. Since gas mixture at core always

TABLE II
GEOMETRIC PROPERTIES OF NISSAN VQ20 ENGINE

Engine: Nissan VQ20, DOHC 24-valve	
Bore X Stroke	76 X 73.3 [mm]
Compression Ratio	9.5:1
No. of cylinders	120 degree V6
Inlet valve open	3 BTDC
Inlet valve close	41 ABDC
Exhaust valve open	49 BBDC
Exhaust valve close	3 ATDC

TABLE III
CHEMICAL PROPERTIES OF N-HEPTANE [3],[4]

Formula	nC_7H_{16}
Molar mass (g/mol)	100.16
Density (g/ml)	0.692
Boiling point (°C)	98
LHV (MJ/kg)	44.5
RON	0
$\Delta_f H°$gas [kJ/mol]	-189.30

TABLE IV
ENGINE CHARACTERISTICS AND MODEL PARAMETERS

Clearance volume	[cm^3]	32.00
Crank radius	[mm]	36.6
Connecting rod length	[mm]	147.7
Swept volume	[cm^3]	332
Combustion efficiency		0.95
Volumetric efficiency		0.95
Polytropic compression exponent		1.335
Polytropic expansion exponent		1.35

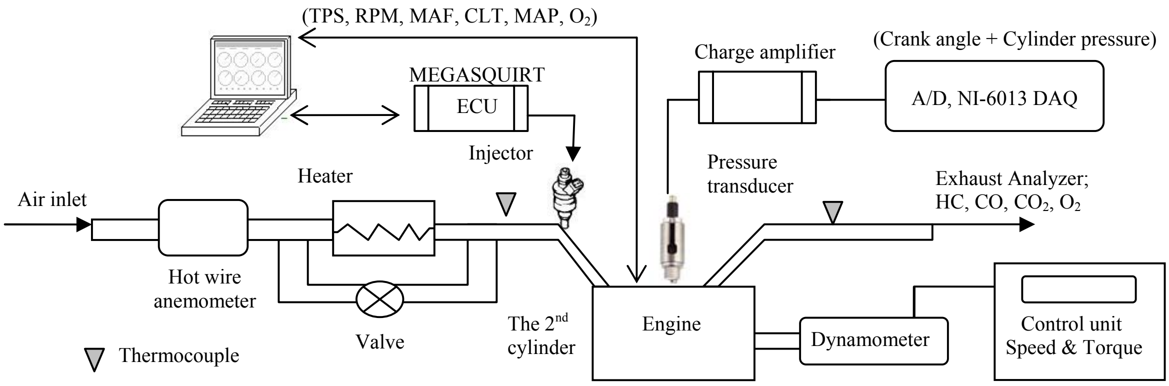

Fig. 1 Experiment layout

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hotter and greater spread of autoignition time than in the cooler [17]. During combustion phase, HCCI model employs only the Wiebe-function option since a turbulent flame model has no role in HCCI combustion [18].

In this study, model to predict pressure and temperature traces during inlet valve close and outlet valve open in HCCI operation were presented. The results were compared with the experiment data. Constants used in the model were fitted corresponding to the data.

II. Experiment Setup

A. Description of Engine

A six-cylinder, four stoke SI engine was utilized in this study. One cylinder of the prototype engine was modified to operate in HCCI mode, while the other 5 cylinders were kept running in the original SI mode. The specification of the engine test cylinder is shown in Table II and n-heptane was fuelled in HCCI mode with its thermal properties shown in Table III.

Two ECUs were performed to control the engine as original SI mode and HCCI mode separately on the selected cylinder. The 2nd cylinder was selected to run in HCCI mode and connected to modified manifold with function to supply A/F mixture separate from original. Heater and bypass valve were used to control intake temperature and addition injector fuel n-heptane.

The engine was coupled to an eddy current dynamometer (Schenck W230 eddy current dyno) for speed and torque measurement and control. The engine was started and allowed to warm up for a period of 20 minutes. Engine tests were operated at constant speed of 1300 rpm on various intake charge temperature and equivalence ratio. Before running the engine with a new equivalence ratio, it was allowed to run in SI mode as using gasoline in order to keep high temperature in the combustion chamber. The engine coolant and engine oil were maintained at 65°C.

B. Instrument and Signal Condition

To monitor and analyze data efficiently, all of the signal collected by transducers were passed through NI-DAQ6013 and managed by Labview8.2 software. The cylinder pressure was detected by piezoelectric cylinder pressure (Kistler model 6117BF17). The charge output was converted to amplified voltage using charge amplifier (Kislter model 5011B). Coupling with crank angle position signal to trigger the record of cylinder pressure, 40-consecutive cycles during combustion period were sampled with resolution of 0.5°CA.

Pulse width signal for additional injector was controlled by the second ECU, MegaSquirt V3.7 board and Megatune 2.25 software which allow user to monitor and correct engine parameters to match the operating condition. Output pulse width is determined in a two dimensional lookup-table with engine speed and air flow rate (Signal from MAF, manifold air flow sensor) as parameters. The final pulse width is modified by intake air and coolant temperature.

According to the collected cylinder pressure for each operation point, Heat release rate was calculated from the relation of pressure and crank position [2].

III. Engine Model

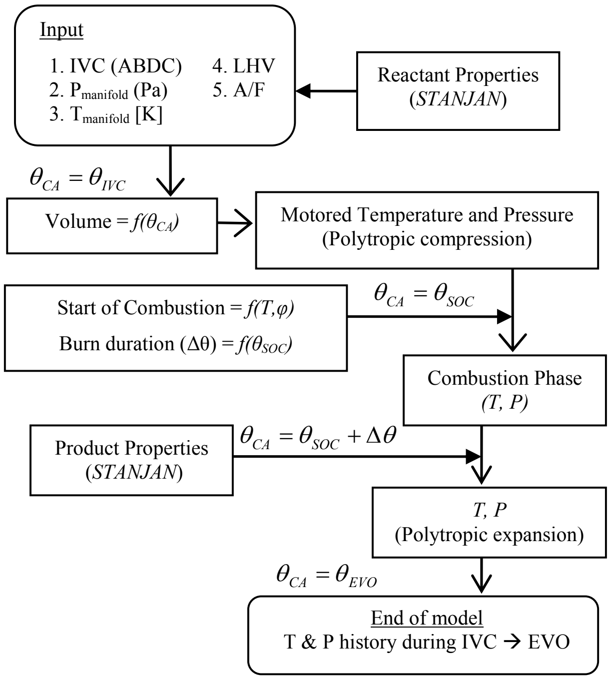

Fig. 2 Algorithm flow chart

Theory background for dealing with combustion in internal combustion relate to knowledge of thermodynamic and combustion mechanic as following. Model algorithm is displayed in Fig. 2. At the beginning of calculation, engine geometry has been accounted. Cylinder volume is related to the rotation of crank shaft as [12]-[14].

$$V(\theta) = V_{Cl} + \frac{\pi B^2}{4}\left(l + a - a\cdot\cos\theta - \sqrt{l^2 - (a\cdot\sin\theta)^2}\right) \tag{1}$$

A. Inlet Valve Close to Start of Combustion

The pressure and temperature histories during compression are calculated using a polytropic compression from IVC to SOC. They are displayed as function of crank angle with coefficient n_c =1.3 [15], [16].

$$T_{cyl}(k,\theta) = T_{IVC}(k)\left(\frac{V(\theta_{IVC})}{V(\theta)}\right)^{n_c - 1}$$, and

$$P_{cyl}(k,\theta) = P_{IVC}(k)\left(\frac{V(\theta_{IVC})}{V(\theta)}\right)^{n_c} \tag{2}$$

After finish combustion phase, polytropic expansion like (2) is performed to simulate the phenomena in expansion stroke.

B. Start of Combustion

Almost of the prediction in SOC based on Arrenius equation, SOC is a function of temperature, pressure, concentration of mixture and empirical coefficient as shown [15];

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$$AR = \int_{t_{ivc}}^{t_{soc}} \beta([F]_{ivc},[O_2]_{ivc})\, p(t)^n \cdot$$

$$\exp(-\frac{E_a}{RT_c(t)})[F](t)^c[O_2](t)^d\, dt \tag{3}$$

It implies the accumulation of radicals (AR) from stable species which prompt to oxidation. Integration from inlet valve close until the combustion is imitated corresponds to a critical value of the concentration of radicals. Since only 1% of fuel is burnt which at point of initial of combustion. The chemical concentration of fuel and oxygen can be considered constant throughout the compression stroke before ignition and equal to the concentrations at inlet valve close.

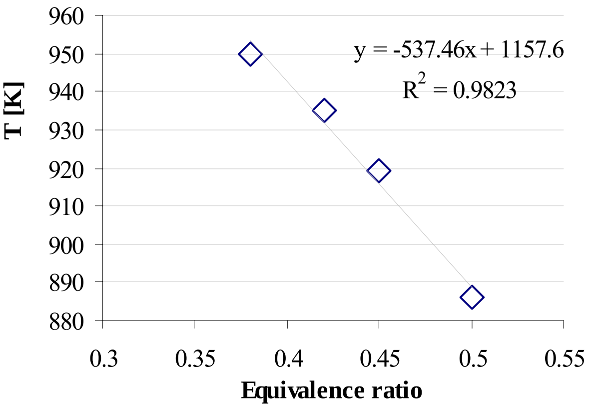

Fig. 3 T_{SOC} and φ at which 1% heat release occurs and ignition line was least squares fit to the data φ

According to the experiment data in Fig.3, SOC depends on equivalence ratio and intake charge temperature. After inlet valve close, the charge temperature and pressure are increasing as compression stroke until meet the autoignition point. Since lower equivalence ratio requires higher intake charge temperature to reach more temperature at compression stroke, especially at low CR engine, T_{ivc} must be increased to meet autoignition criteria. This relation refers to the line that temperature and equivalence ratio cross a specific line. SOC is simply as shown below;

$$T_{soc}(\theta) = a1(\varphi) + b1\,; \tag{4}$$

Where constant *a1* and *b1* are -537.46 and 1157.6 respectively refer to the experiment results. The left and right side of (4) will be equal as increasing of temperature in compression stroke and then combustion is assumed beginning. SOC could be rewritten as

$$T_{IVC}(k)\left(\frac{V(\theta_{IVC})}{V(\theta_{SOC})}\right)^{n_e-1} = a1(\varphi) + b1 \tag{5}$$

$$\theta_{SOC} = f\left(T_{IVC}(k), \varphi, a1, b1\right) \tag{6}$$

C. Combustion Duration, (Δθ)

Combustion duration depends on SOC angle as

$$\Delta\theta(k) = a2 \cdot \theta_{SOC}(k) + b2 \tag{7}$$

Corresponding to [2] and the experiment results, replaces *a2* and *b2* as -81 and 0.5 respectively. The longer combustion duration is result from the more retard of SOC.

D. Start of Combustion

From SOC, temperature rise due to combustion and temperature change depends on LHV (Low heating value) of fuel, A/F, combustion efficiency as well as specific heat.

$$T_{CA50} = T_{soc} + \Delta T \tag{8}$$

$$\Delta T = \frac{\eta_c Q_{LHV}}{c_v} \frac{1}{1 + A/F}(x_b) \tag{9}$$

Air and fuel mixture through chamber will not burn at the same time and rate. This has been considered in double-Wiebe function combustion model which a fuel burn fraction at reduced rate can be described as [17]

$$x_b = (1-\alpha)\left\{1 - \exp\left(-w\left(\frac{\theta-\theta_0}{\Delta\theta}\right)^{m+1}\right)\right\}$$

$$+\alpha\left\{1 - \exp\left(-w\left(\frac{\theta-\theta_0}{K\Delta\theta}\right)^{m+1}\right)\right\} \tag{10}$$

Where w is derived from the Wiebe function between specific burn fractions of 0.1 and 0.9.

$$w = w_{10-90}$$

$$= \left[\left\{\ln\left(\frac{1}{(1-0.9)}\right)\right\}^{1/m+1} - \left\{\ln\left(\left(\frac{1}{1-0.1}\right)\right)\right\}^{1/m+1}\right]^{m+1} \tag{11}$$

This step is coupled with ideal gas law in order to predict combustion pressure. Thermal properties uses in this step were calculated by STANJAN software.

IV. Results and Discussions

A. HCCI Operation

Pressure and temperature history during IVC and EVO were investigated. According to the experiment shown in Fig.4, pressure traces were collected directly and found that pressures

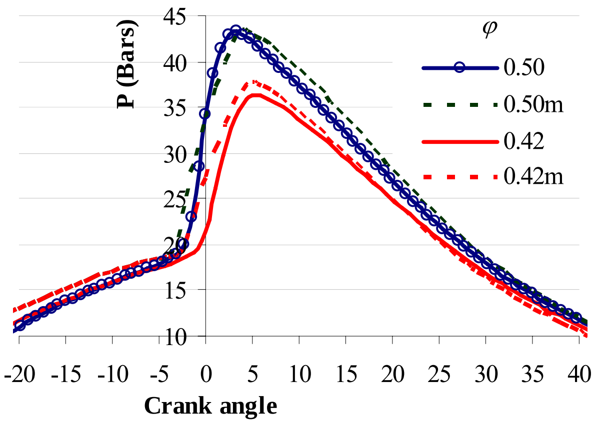

Fig. 4 Predicted and experimental pressure history

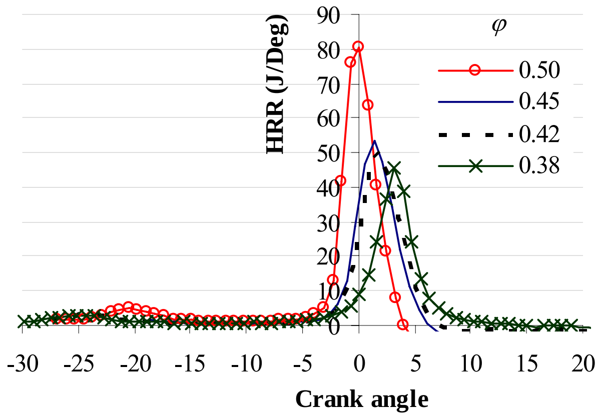

Fig. 6 Heat release rate at variance equivalence ratio

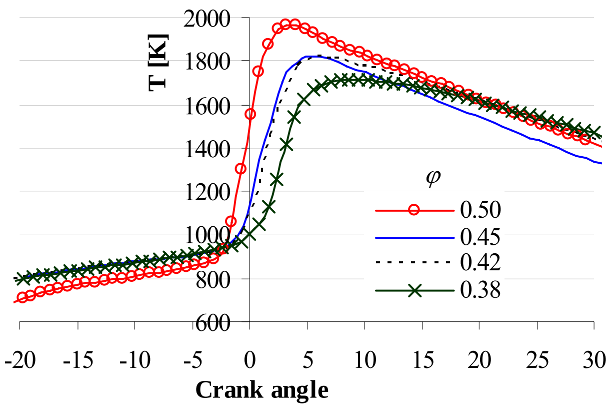

Fig. 5 Temperature history derived from ideal gas law

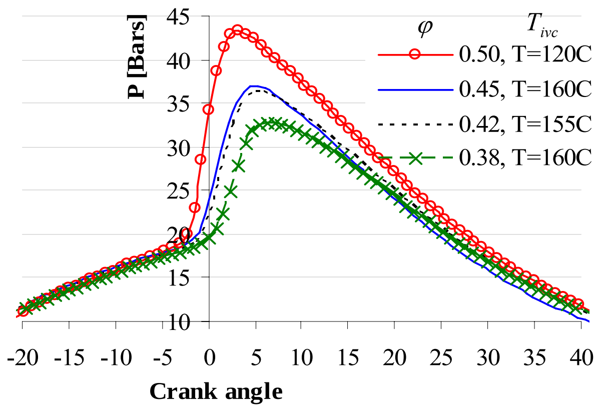

Fig. 7 Predicted combustion pressure history

were raising until SOC at few degrees before TDC. Pressures at SOC were around 17 to 18 bars and valid the polytropic assumption in the model. Regardless amount of equivalence ratio, the location of SOC were quite similar since intake charge temperature were adjusted to meet the highest torque at varied conditions. Required intake charge temperature could be lower as increasing in equivalence ratio. Temperatures range from 160 to 120°C for equivalence ratio of 0.35 to 0.50 respectively.

During combustion phase, the maximum pressure depended on amount of equivalence ratio and higher equivalence ratio cause increase in peak pressure. Maximum pressures were 33, 36, 37, and 43 bars at equivalence ratio of 0.35, 0.42, 0.45, and 0.50 respectively. Collected pressure history coupled with the relation of cylinder volume was also converted to temperature history using ideal gas law. Temperature history at equivalence ratio of 0.5 was shown in Fig. 5 as peak pressure and temperature were the same position.

PRR describes as an index to define the intensity of combustion roughness, in this study; the “knock combustion” replied the maximum PRR exceeds 10 bars/CA [14]. Hence, the equivalence ratio kept smaller than 0.50 or is the upper limit in this study to maintain maximum PRR less than the limit. Under the condition of higher equivalence ratio, the ignition of premiixed mixture were start continuously and implied on increase in PRR that combustion occurred close to constant volume. After combustion period, the pressure reduce undergo expansion stroke.

Combustion durations implied form heat release rate shown in Fig.6. They were used to adjusted (7) as more advance of SOC related to TDC, combustion duration will shorter. Pressure trace of 0.50 equivalence ratio showed the earliest in SOC and combustion duration was 4 degrees till CA90. At equivalence ratio of 0.38 expressed the longest burn duration as the most retard in SOC compare with others. According to SOC, peak pressure location shift to TDC as increasing in equivalence ratio. These refer to shorter combustion duration and led to higher in PRR.

B. Model Results

Simulation via model with STANJAN software facility, temperature and pressure at SOC was predicted by model. Mixture component and quantity were affected by the equivalence ratio and manifold temperature. At first, thermal properties and especially enthalpy of mixture at specific condition, SOC points were obtained. The model began at inlet valve close; thermal properties of mixture and thermal condition were given. Pressure increasing behaves polytropic until meet SOC requirement as (5) and (6) while the piston angle rotates approach TDC.

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Charge temperature and equivalence ratio were used as the index for determine SOC point. Even (4) showed the simply relation corrected by experiment data. They are similar to Arrhenius equation which combustion start after account the accumulation of temperature while others variable assume constant. Equivalence ratio is considered like concentration of reactants. They increase the amount of accumulated radicals in the combustion chamber to meet autoignition criteria.

Pressures at any equivalence ratios were about 17 bars similar to experiment results and correspond engine geometry. Considering double-Wiebe function, fitting parameters of slower combustion, α, *m*, and *K* were 10, 0.4, and 0.25 respectively.

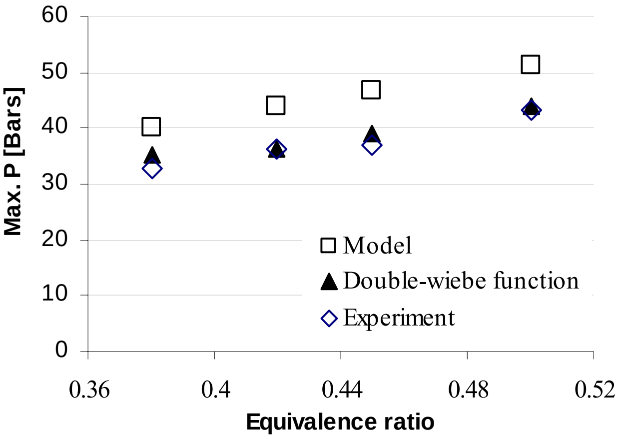

Fig.8 Maximum pressure at variance equivalence ratio

Thermal properties of cylinder mixture were updated by STANJAN. Defined the product components in correspond with specific volume and enthapy of previous run or reactant, STANJAN could determine quality and quantity of final product. Predicted peak pressures were obtained and found that were higher than experiment results displayed in Fig.8. Without double-Wiebe function, model results showed over prediction in combustion pressure at the mean of 22.22% difference. As combustion is assumed occur instantaneously and no heat loss. Also the wear of piston, rings and cylinder affect the volume at any position as leakage. Predicted peak pressures were higher than experiment results. Successively double-Wiebe function was performed. Almost peak pressures were smaller and close to experiment result with the mean of 5.82% difference.

V. Conclusion

HCCI operation at equivalence ratio 0.38 to 0.50 have been run and investigated. Experiment results were analyzed and fitted for corrected the model. Predicted SOC refer to experiment as *a1* and *b1* were -964.8 eland 1231.7 respectively. Fitting parameters of slower combustion, α of 10 and *K* of 0.25 were used in the model. Combustion phase coupled with double-Wiebe function helped model results close to experiment at 5.82% difference. The model calculated temperature and pressure trace during IVC and EVO interval.

Single zone model with double-Wiebe function showed good accuracy of calculation in SOC and the highest pressure and temperature in combustion phase. The model could be possibly incorporated with control software to predict the occurrence of SOC in HCCI operation since the computation time is short and the required information such as intake charge temperature could be obtained on line.

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