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Pressure Distribution, CO and HC Emission on the Equivalence Ratio Variation of Homogeneous Charge Compression Ignition (HCCI) Engine Simulation

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Abstract: HCCI combustion mode is a combination of the modes of Compression Ignition (CI) and Spark Ignition (SI). A very short duration of combustion in HCCI resulted in faster pressure increases than that at the SI engine and even on the Compression Ignition Direct Injection (CIDI) engine. This research was aimed at finding the pressure distribution and CO-HC emission of the engine. They were predicted on two models, i.e., single zone and multi zone models. Multi zone model divides the cylinder into ten different zones and 3 K stratification temperatures. Two reaction mechanisms were implemented, i.e., detail mechanism and reduced mechanism. Thermodynamic equations of the species involving in combustion reaction were presented in polynomial function of specific heat coefficient, enthalpy and entropy within the temperature range. Reaction mechanism was determined based on arhennius coefficient and state equation was presented in multi-fluid ideal gas where the pressure and density of reactant were presented in the summations of pressure and density of species. The rate of progress reaction was defined as the difference between forward rates and reverse rates and the rate of progress species was defined as the summations of all the rate progress species involved in the reaction. Both models were simulated on the crank angles of 1650-1700 referring to the experiments of the other researchers. The simulation was conducted on five variations of equivalence ratio and was carried out using kinetic reactions based software. The results were presented in graphics comparison of experiment and simulation. Pressure distribution of the experimental and the simulation results on single zone model and multi zone model showed the same tendency on the reduced mechanism results in the higher equivalence ratio. The detailed mechanism on a single zone model gave closer results to the experimental one compared with the reduced mechanism. While CO-HC emission of the experiment under reduced mechanism simulation seemed fit quite well on the equivalence ratio of approximately 0.2 they, however, deviated far at higher equivalence ratio because the fuel, theoretically, gets enough air to burn perfectly.

Key words: Combustion modeling, simulation, HCCI, Compression Ignition Direct Injection (CIDI), thermodynamic equations, experiment

INTRODUCTION

Combustion processes involve species composition of the mixture changes with time and a very large increase in temperature due to the heat release from the excess molecular bond energy. They are complex phenomena that depend upon interrelated processes of thermodynamics, fluid mechanics, chemical kinetics, heat and mass transfer and turbulence. Solutions of combustion problem require theoretical formulation and combustion modeling. Components of theoretical model are governing equations, initial conditions, boundary condition, equations of state, thermodynamic and transport properties, kinetic data, empirical input, material properties and structural characteristics. The governing equations are linked to all other components that make the problem more complicated (Kuo, 1986; Roger, 1985).

However, with the advancement of computer and numerical techniques, the objective of combustion modeling can be achieved. This research presented combustion modeling in Homogenous Charge Compression Ignition (HCCI) engine. HCCI is an alternative system of combustion in an internal combustion engine. HCCI can be seen as a combination of Compression Ignition (CI) and Spark Ignition (SI) combustion system. Similar to the fuel injection system of SI, air and fuel are mixed in advance to obtain a homogeneous mixture before being injected into the

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combustion chamber. But in the absence of spark plugs, the beginning of the burning is caused by the compression of high temperature such as in the burning system of CI. HCCI has the potential to reduce the problems that occur on the current internal combustion engine it is seen as a step forward that offers higher efficiency of the system and lower emissions of CI systems.

The launch of the car with a mixed system of diesel HCCI-Mercedez E320 CDI in 2004 and the debut of the Vauxhall Vectra 2.2 that uses HCCI SI-alloy system in 2009, shows that HCCI technology has evolved from a conceptual design into commercial applications (Su, 2010). Most major benefits of HCCI technology are the lack of production of NOx and Particulate Matter (PM) until it almost reaches zero while maintaining high thermal efficiency (Tzanetakis, 2007). Research on new model of heat transfer employed in multi zone chemical kinetics model to estimate convective heat transfer of HCCI engines more accurately have been developed Elaheh (Neshat and Saray, 2014).

Unfortunately, there are some of the challenges associated with the use of an HCCI that must be addressed. One of the most important is the lack of control over the time of beginning and duration of burning. Combustion control can only be done indirectly throughout equivalence ratio, compression ratio, Exhaust Gas Recirculation (EGR), octane number and other indirect control parameters. A very short combustion time resulted in combustion pressure increases rapidly. This can lead to knocking, if the fuel mixture is too rich but if the fuel mixture is too poor, the engine will experience misfire (Su, 2010). Therefore, mixture preparation and control strategies on the HCCI engine are very important.

Engine modeling has a contribution in the development of machines such as identifying key variables, so that it can reduce the cost of experiments, predict the behavior of engine in the range of design and operating variables and provide a rational basis in the maintenance (Heywood, 1988). Aldawood *et al.* (2011) performed HCCI engine test and conducted a model using Stochastic Reactor Model (SRM) with reduced mechanism that composed of 157 species and 1552 reactions. Pressure distribution was used to optimize the model by using a function optimization. The results of the pressure of optimization functions were enough to approach the results of experiments. Moreover, a thermodynamic model has been developed to consider the gas composition resulting from the combustion process and the specific heat temperature dependency of the working fluid. The influence of the compression ratio, ambient temperature, equivalence ratio, engine speed and the compressor isentropic efficiency on the performance of the HCCI engine had been investigated (Djermouni and Ouadha, 2014).

MATERIALS AND METHODS

Combustion modeling on HCCI engine was performed by using two types of modeling-single zone and multi zone on two reaction mechanisms, i.e., detailed mechanism consisting of 1034 species and 4236 step reactions and reduced mechanism consisting of 32 species and 55 step reactions. Multi zone model divides the cylinder into 10 different zones and 3 K stratification temperature (Tzanetakis, 2007) with the volume of the core zone of 20% and the ratio of geometric 0.8.

Thermodynamic data of species which react in a combustion were expressed in the form of polynomial functions, where there are 14 polynomial coefficients for two temperature range; 7 coefficients for each temperature range for each species. The thermodynamic data followed the following polynomial functions (Chemkin 2008):

$$\frac{C_{pk}^{0}}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \quad (1)$$

$$\frac{H_k^0}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T} \quad (2)$$

$$\frac{S_k^0}{R} = a_1 \ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7 \quad (3)$$

Where:

T = Temperature
a = Polynomial coefficients
R = Gas constant
$C_p°k$, $H_k°$ and $S_k°$ = Specific heat capacity at constant pressure, enthalpy and entropy of kth species respectively on the standard state of 1 atm

Reaction mechanisms are written in 3 arrhenius coefficients which are temperature factor, pre-exponential factor and energy activation factor that showed how fast the reaction would take place. Reaction rate constants at step i is given by Kuo (1986), Bendu and Murugan (2014):

$$k_i = A_iT^{\beta_i}e^{\left(-E_i/RT\right)} \quad (4)$$

where, A_i, β_i, E_i are arrhenius coefficients; pre-exponential factor, temperature exponent and activation energy. The production rate (ω_k) of the kth species can be written as

a summation of the rate of progress variables for all reactions involving the kth species while the rate of progress variable q_{ki} for the ith reaction is given by the difference of the forward and reverse rates as shown in Eq. 5 and 6 (Chemkin, 2008):

$$\dot{\omega}_k = \sum_{i=1}^{I} \nu_{ki} q_{ki} \quad (5)$$

$$q_{ki} = k_{fi} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{ri} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \quad (6)$$

Where:

X_k = Molar concentration of the kth species
k_{fi} and k_{ri} = The forward and reverse rate constants of the ith reaction
ν_{ki}' = Stoichiometric coefficient of the reactants
ν_{ki}'' = Stoichiometric coefficient of products in the reaction of k-i
ν_{ki} = Difference between ν_{ki}' and ν_{ki}''

The rate-of-progress of a reaction is evaluated by default, using the concentration of each reactant or product species raised to the power of its stoichiometric coefficient ν_{ki}. Thus, the rate-of-progress of a reaction that includes species A with a coefficient of 2 will be second-order with respect to the concentration of A. Changing the amount of species k is defined by Chemkin (2008):

$$\rho(^{dY_k}/dt) = \omega_k W_k \quad (7)$$

Where:

ρ = The density
Y_k = The mass fraction of species k
k and W_k = The molecular weight of the species k

The state equation for multi-fluid ideal gas was used where the pressure and density are expressed as the following:

$$p = \sum_{k=1}^{K} [X_k] R T_k \quad (8)$$

$$\rho = \sum_{k=1}^{K} [X_k] W_k \quad (9)$$

Fuel for this combustion processes was Primary Reference Fuels (PRF) 40 which consisted of 40% iso-octane and 60% n-heptane. The simulation was conducted on five variations of equivalence ratio and was carried out using kinetic reactions based software. Initial value for temperature and pressure was 370 K and 1 bar. Simulations conducted since the Intake Valve Closes (IVC) until the Exhaust Valve Open (EVO) and engine rotation was 1,200 rpm on crank angle 165°-170°. The parameters of the engine, fuel and simulated parameters were adapted from (Aldawood *et al*., 2011). The simulation results would be compared with their results.

RESULTS AND DISCUSSION

Pressure distribution and CO and HC emission graphics as the results of the simulation on five variations of equivalence ratio can be seen in Fig. 1-5. Each figure presents 4 curves, i.e., SR is for single zone, reduced mechanism, SD is for single zone, detailed mechanism, MR is for multi zone, reduced mechanism and experiment.

Pressure distribution: Pressure distribution on reduced mechanism (SR and MR) shows higher maximum pressure than that of experimental result. It means that the rate of heat release is faster. However, as the equivalence ratio increases, the curves seem almost fit well given the better prediction.

On the same mechanism, the reduced mechanism, multi zone Model (MR) did not give many different results

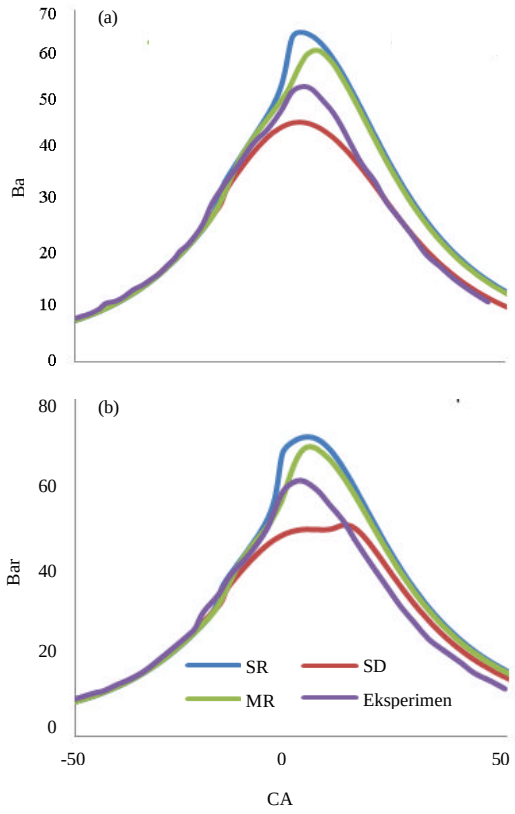

Fig. 1: Pressure distribution on equivalence ratio of: a) 0.19 and b) 0.21

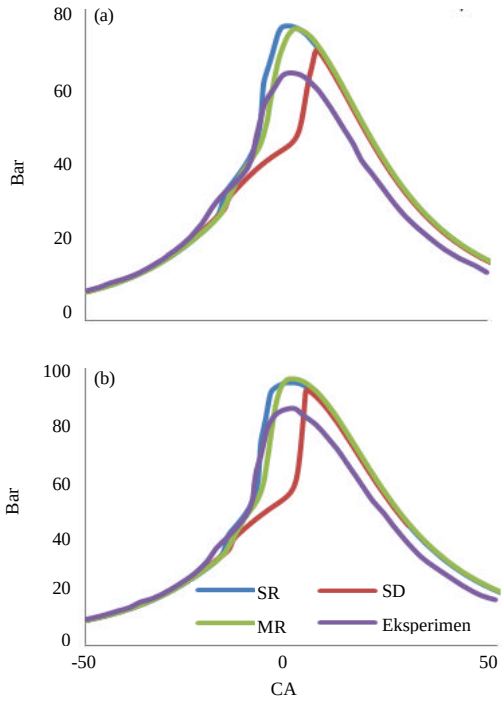

Fig. 2: Pressure distribution on equivalence ratio of: a) 0.26 and b) 0.29

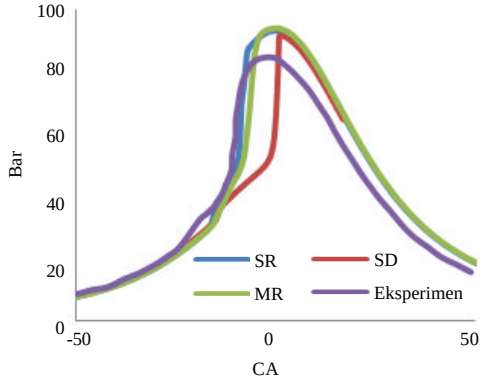

Fig. 3: Pressure distribution on equivalence ratio of 0.32

from the single zone (SR) Model because the mass fraction in the gap zone was not large enough to hold back the rate of heat release from the fast temperature increase. In general, all the graphics of pressure distribution on the crank angle give a representative result as the maximum pressure achieved on the crank angle was nearly zero.

However, on the detailed mechanism there exist ignition delays as a second-stage ignition could be seen on the curve especially on the equivalence ratio above 0.21. This can be interpreted from the ignition delay

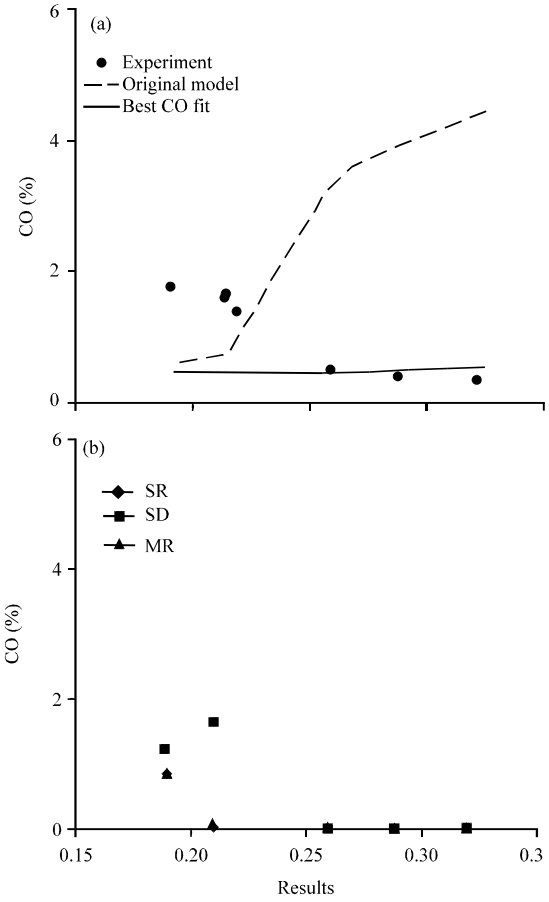

Fig. 4: Prediction of: a) CO emission on experiment (1200 rpm-PRF40) and b) Simulation results

theory for HCCI combustion. As the equivalence ratio increases, the HCCI ignition delay must be decreased to keep up with shorter cycle times, thus a second ignition is needed (Tian, 2013).

CO and HC emission: Figure 4 and 5 predict the emission of CO and HC on the equivalence ratio variation. Hydrocarbon and carbon monoxide emission is one of the challenges topics on HCCI researches (Swapnil *et al*., 2014). They both showed that under reduced mechanism both single zone and multi zone models could not provide information on emissions as the increasing of equivalence ratio. The concentration of CO and HC emissions is nearly zero. A large number of intermediate reactions which were skipped on the reduced mechanism might be the reason why the rate of reaction became very fast so that there was no CO and HC formation. Detailed mechanism (SD) gave good results in the prediction of the emission of CO and HC on the equivalence ratio of approximately 0.2. As the increasing of the equivalence ratio, CO and HC

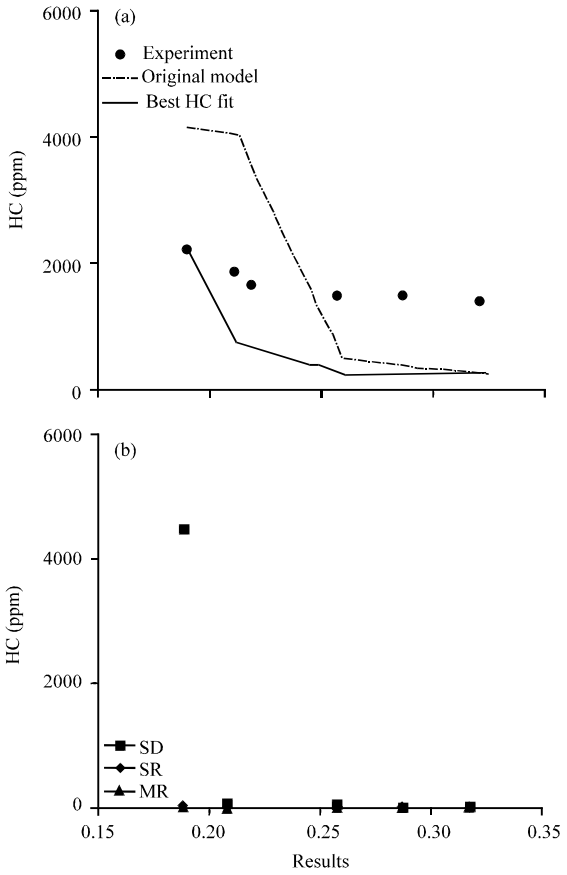

Fig. 5: Prediction of: a) HC emission on experiment (1200 rpm-PRF40) and b) simulation results

prediction deviated far from the experiment result. The value was approaching zero because the fuel got enough air to burn perfectly over the increasing of equivalence ratio. The mixture ishomogenous in nature, so that there is no local rich or lean zone. In term of modelling zone, the multi zone Model (MR) has also shown no effects due to the small mass fraction on the crevice zone. Therefore, the result was almost similar to the single zone model.

Combustion modelling that involves many governing equation derived simulation processes from incorporating computer simulation. The simulation results indeed helped to interpret and understand the combustion phenomena and establish the influence of certain parameters in combustion processes by conducting parameters studies.

CONCLUSION

Governing equations on combustion modeling are very complex and computer simulation really facilitated to obtain solutions. The simulation and experiment results on the HCCI engine showed the same tendency particularly on lower equivalence ratio. The simulation on the single zone and multi zone modeling also demonstrated the same trend.

The reduced mechanism generated greater maximum pressure than that from the experimental results due to high rate of heat release on the model and would tend to match over the increasing equivalence ratio. The detailed mechanism generated lower maximum pressure than that from the experimental results on the equivalence ratio of 0.19 and 0.21. Under the reduced mechanism higher the equivalence ratio promoted similar maximum pressure between the experimental and simulation results. The detailed mechanism experienced an ignition delay compared to the reduced mechanisms that run very fast. The experiment and the reduced mechanism simulation did not suffer any second-stage ignition within the equivalence ratio of 0.19 and 0.21.

CO and HC emission could not be well predicted in the reduced mechanism simulation. Higher equivalence ratio gave more air to burn so that CO and HC emission became zero. The detailed mechanism simulation could only predict CO and HC emission on equivalence ratio of about 0.2. Higher equivalence ratio provided the same failure as on the reduced mechanism simulation.

Implementation of HCCI on alternative fuel particularly sustainable bio fuel was one of future research that need further investigation as there are no existing computer simulations models for the large molecules characteristic of biodiesel fuels, computational models can be used to predict HCCI ignition timings for any of these cases. The possibility of using gas mixtures that almost similar to the bio fuel compositions can be a consideration.

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