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Predicting the Combustion Behaviour of a Diesel HCCI Engine Using a Zero-Dimensional Single-Zone Model.

A. Aziz Hairuddin[1, 2*], Talal F. Yusaf[2], Andrew P. Wandel[2]

[1.] Department of Mechanical and Manufacturing Engineering, Faculty of Engineering, Universiti Putra Malaysia, Malaysia.

[2.] Faculty of Engineering and Surveying, University of Southern Queensland, Australia.

Abstract

Homogeneous charge compression ignition (HCCI) engines use a new mode of combustion whose technology has not matured sufficiently to be commercialized. There are several challenges in developing HCCI engines: auto-ignition control of the mixture, achieving a cold start and controlling knock at high load operation. In principal, HCCI engines have no spark plug or fuel injector to control the combustion: auto-ignition occurs in multiple spots once the mixture has reached its chemical activation energy. The chemical reaction of the mixture is influenced by changing input parameters such as: intake temperature, equivalence ratio and fuel type. A zero-dimensional single-zone model is used to investigate the combustion behaviour of a diesel engine operating in HCCI mode, with n-heptane used as a surrogate fuel for diesel. The combustion phasing is predicted in accordance with the experiment, with higher in-cylinder peak pressure. This paper will study methods of controlling the auto-ignition timing through hydrogen addition and by altering the intake air temperature and equivalence ratio. The auto-ignition timing changes with the change of all those factors, where the combustion phasing is advanced by increasing all the parameters.

Keywords: Diesel HCCI, zero-dimensional, single-zone

1. Introduction

Internal combustion (IC) engines have been extensively used to generate power for various applications throughout the world: car engines, power generation plants and ships. The emissions generated from these sectors have a high impact on the environment so alternatives have been investigated worldwide to achieve low emissions levels.

A homogeneous charge compression ignition (HCCI) engine is a relatively new technology even though it was initially investigated by Onishi et al. for gasoline engines [1]. HCCI engines are reported to have high efficiencies relative to spark ignition (SI) engines, and approach the efficiency of compression ignition (CI) engines due to high compression ratio (CR) and fast combustion [2, 3] and also have the ability to operate using a wide range of fuels [4]. In addition, HCCI can be implemented in any engine configuration: automobile engines, stationary engines, high load engines or small size engines [5, 6]. However, HCCI engines have difficulties: controlling the auto-ignition and heat release rate at high load operation, achieving cold start, and controlling knock [7, 8]. One of the major challenges in HCCI engines is the control of the auto-ignition timing of the mixture because there is no spark plug or fuel injector to control the start of the combustion. The problem becomes more prominent when the engine experiences dynamic loads, which cause the auto-ignition point to be different for different engine operating loads.

The effects of equivalence ratio, intake temperature and other operating parameters to control the auto-ignition timing have been widely investigated [9]. However, hydrogen addition to the diesel HCCI engine seems to be a rare case. Hydrogen addition is able to increase the engine efficiency by a significant margin [10].

Various researchers have investigated the HCCI engine experimentally and numerically. A numerical zero-dimensional model is well accepted by most researchers [8, 11] and can be applied to HCCI engines. The authors are currently developing a complex HCCI engine model, starting with a zero-dimensional model before implementing turbulence and mixing models. This paper reports the first stage (zero-dimensional model): validation and some preliminary results for different intake air temperature, different equivalence ratio and the effect of hydrogen addition.

Section 2 of this paper describes the mathematical model used in the simulation, followed by the validation of the model, comparison of the predicted result with experiment for different operating conditions. Finally, the methods to control the auto-ignition point are discussed.

2. Model Formulation

The zero-dimensional model in this paper is for an open system, initially developed by Assanis and Heywood [12]. The results presented here focus on the combustion behaviour between inlet valve open (IVO) and exhaust valve open (EVO) because the emissions generated in the exhaust gas after EVO are not of interest in this study. It was assumed that the working

* Corresponding author:
Phone: (+61) 7 4631-1381
Email: AbdulAziz.Hairuddin@usq.edu.au or aziz8411@eng.upm.edu.my

fluid is an ideal gas and the thermodynamic properties are uniform throughout the combustion chamber.

2.1 Conservation of mass

The continuity equation is governed by the mass flows in and out of the system:

$$\frac{dm}{dt} = \sum_j \dot{m}_j \tag{1}$$

where $\dot{m}$ is the mass flow rate, m is the mass and the subscript j is the component species in the mixture.

2.2 Conservation of species

To accurately model combustion in HCCI engines requires sufficiently detailed chemical reaction mechanisms; an n-heptane reduced mechanism [13] was used here to simulate diesel combustion. The chemical properties of this surrogate fuel (e.g. cetane number) are similar to conventional diesel. The mechanism consists of 160 species and 770 elementary reactions. The change of mass fraction of each species due to chemical reactions is governed by:

$$\frac{dY_i}{dt} = \frac{\dot{\omega}_i W_i}{\rho}, i = 1, \ldots, n \tag{2}$$

where Y_i is the mass fraction of each species, $\dot{\omega}_i$ is the molar production rate of the ith species, ρ is the density and n is the total number of species.

2.3 Conservation of energy

The energy equation was derived from the first law of thermodynamics for an open system:

$$\frac{dmu}{dt} = \frac{dQ}{dt} - P\frac{dV}{dt} + \sum_j \dot{m}_j\, h_j \tag{3}$$

where u is the specific internal energy, Q is the net heat transfer, P is the pressure, V is the volume and h is the specific enthalpy. Manipulating (3) results in

$$m\frac{dh}{dt} = \sum_j \dot{m}_j\, h_j + \frac{dQ}{dt} + V\frac{dP}{dt} - h\frac{dm}{dt} \tag{4}$$

The change of enthalpy is determined by assuming a single phase, multi-component mixture of ideal gas

$$\frac{dh}{dt} = C_p\frac{dT}{dt} + \sum h_j \frac{dY_j}{dt} \tag{5}$$

where C_p is the specific heat at constant pressure. The differential form of the ideal gas equation, $PV = mRT$, is

$$\frac{\dot{R}}{R} = \frac{\dot{V}}{V} + \frac{\dot{P}}{P} - \frac{\dot{T}}{T} - \frac{\dot{m}}{m} \tag{6}$$

where the rate of change of the universal gas constant, $\dot{R}$ is given by

$$\frac{dR}{dt} = \sum \frac{R_u}{\bar{W}}\frac{dY_j}{dt} \tag{7}$$

with $\bar{W}$ the mean molecular weight. Substituting (7) into (6) yields

$$\dot{P} = P\left[\frac{\sum_i \frac{R_u}{W}\frac{dY_i}{dt}}{R_u/\bar{W}} + \frac{\dot{m}}{m} + \frac{\dot{T}}{T} - \frac{\dot{V}}{V}\right] \tag{8}$$

Finally, the change in temperature is obtained by substituting (8) into (4):

$$\frac{dT}{dt} = \frac{1}{Cp - \frac{Pv}{T}}\left[-\left(\sum H_i - \frac{Pv\sum_i R_u/W}{R_u/\bar{W}}\right)\frac{dY_i}{dt} - \frac{\dot{m}}{m}\left(h_j - Pv\right) + \frac{1}{m}\left(\sum \dot{m}_j h_j - P\frac{dV}{dt} + \frac{dQ}{dt}\right)\right] \tag{9}$$

In addition, the pressure at each time step is obtained using the ideal gas equation:

$$P = \rho T\frac{R_u}{\bar{W}} \tag{10}$$

2.4 Heat transfer

Heat is transferred to the cylinder wall through convection and radiation, and in this case, the radiation effect is neglected. The heat transfer model is based on the modified Woschni equation by Chang et al. [14]. The radiation heat transfer is neglected because the effect on HCCI engines is very small, due to low soot and low temperature combustion [14, 15].

2.5 Gas exchange process

A gas exchange process takes place when both inlet and exhaust valves are open. One-dimensional, steady state, isentropic flow is used to model the gas exchange process [16].

3. Results and Analysis

The model was validated against experimental data [17], where the HCCI engine was run by using n-heptane as a fuel with port fuel injection, and zero-dimensional modelling [17]. The engine parameters used in this simulation are shown in Table 1.

The fuel was injected at the inlet manifold. To account for mixing effects, the effective intake mixture temperature was set to be higher than the intake temperature: the difference was 20°C [17]. Therefore, the intake temperature for the zero-dimensional model in this study was increased to 333K for the intake temperature of 313K.

The simulation result is compared with the experimental data in Fig. 1. The in-cylinder peak pressure is slightly higher than the experiment due to the limitation of the zero-dimensional single-zone model: it was assumed that the entire combustion chamber is homogeneous. Overall, the combustion phasing is in good agreement with the experimental data, demonstrating that the single-zone model is suitable for use in HCCI engine simulations.

Table 1 Engine parameters used in the simulation [17]

Cylinder bore	82.55 mm
Stroke	114.3 mm
Connecting rod length	254 mm
Compression ratio	10
Engine speed	900 rpm
Inlet valve open (IVO)	10° CA ATDC
Inlet valve closed (IVC)	36° CA ABDC
Exhaust valve open (EVO)	40° CA BBDC
Exhaust valve closed (EVC)	5° CA ATDC

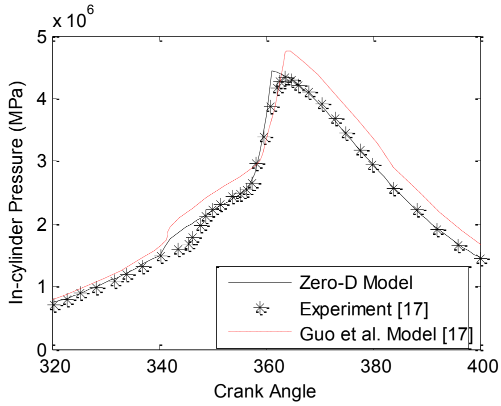

Figure 1 Comparison between single-zone zero-dimensional model with experiment and another single-zone model using modified Woschni heat transfer model [17]. CR=10.0, N=900 rpm, T_{in}=40°C, P_{in}=95 kPa, AFR=50.

3.1 Effect of intake temperature

Intake air temperature is an important factor for controlling the auto-ignition timing of HCCI engines. Different fuels have different auto-ignition points and some of them require pre-heating to achieve good combustion. If methane or natural gas is used as a fuel, the intake air temperature has to be set to at least 400 K to achieve appropriate ignition [18]. Therefore, the intake temperature will affect the auto-ignition point for other fuels as well and increasing the intake temperature will reduce the ignition delay. Thus, the auto-ignition timing can be controlled.

Figure 2 shows that the auto-ignition timing can be advanced once the intake temperature is increased. Results from the current simulation were compared with experimental results [17] in Fig. 2(a) to validate the model over different operating temperatures; results are similar to those in Fig. 1. An increase in air intake temperature will not affect the in-cylinder peak pressure significantly. Note the trend as the intake temperature increases: the predicted in-cylinder peak pressure starts to decrease even though the auto-ignition is advanced, as shown in Fig. 2(b). This trend is also observed in the experiment [17]. This is a good option for control because of the low increase in in-cylinder peak pressure: high peak pressures and advanced auto-ignition will create knocking.

3.2 Effect of equivalence ratio

The equivalence ratio (Φ) is a measure of how much fuel and air is being consumed in the combustion chamber; HCCI engines operate with lean mixtures ($\Phi < 1$). Figure 3(a) shows the validated result of different equivalence ratios compared to the experiment, again showing good agreement.

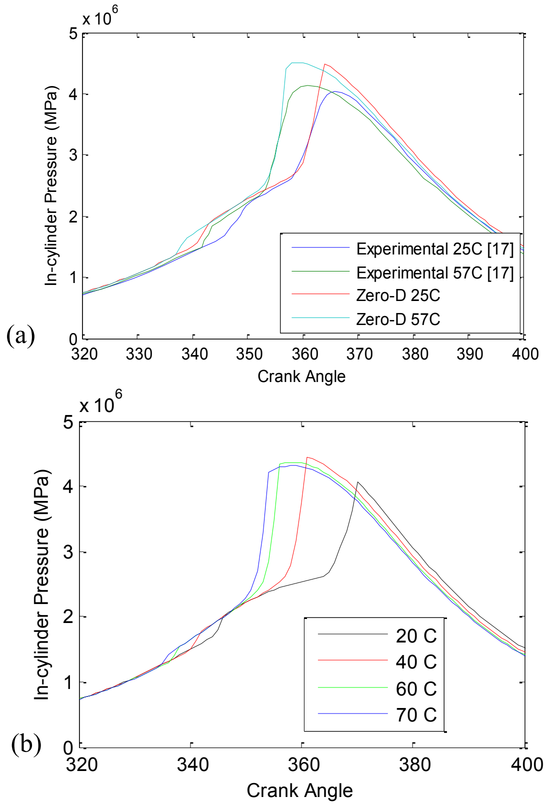

Figure 2 Effect of intake temperature on the in-cylinder pressure: CR=10.0, N=900 rpm, P_{in}=95 kPa, AFR=50 (a) Validated varying intake temperature; (b) Predicted in-cylinder pressure trend.

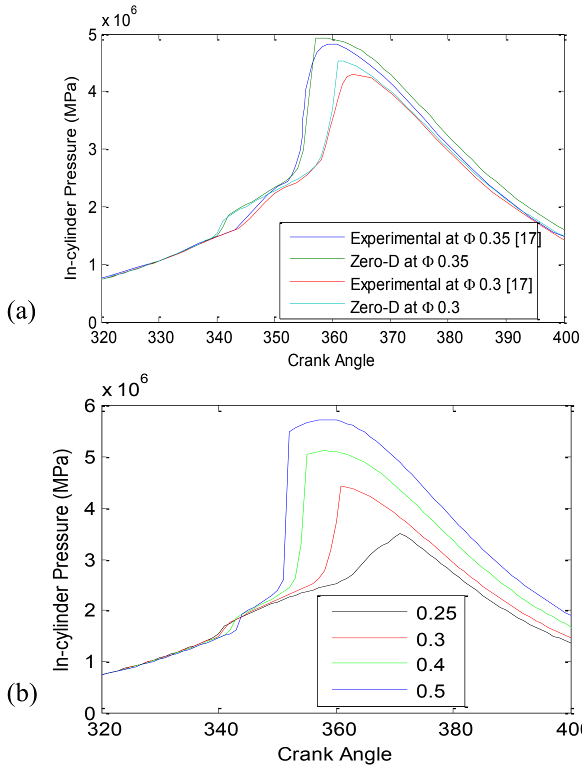

Figure 3 Effect of equivalence ratio on the in-cylinder pressure: CR=10.0, N=900 rpm, T_{in}=40°C, P_{in}=95 kPa (a) Validated varying equivalence ratio; (b) Predicted in-cylinder pressure trend.

Meanwhile, Fig. 3(b) shows the predicted result of increasing the equivalence ratio: an increase in the in-cylinder peak pressure and advancement of the auto-ignition timing. The in-cylinder peak pressure trend keeps increasing with increasing equivalence ratio, which will create knocking. In addition, the start of low temperature reactions (cool flames) is retarded with an increase of equivalence ratio. However, if the mixture becomes too rich, the auto-ignition is advanced significantly and this will lead to knocking: an undesired combustion phenomenon. Therefore, careful tuning is needed to adapt to dynamic engine loads.

3.3 Predicted effect of hydrogen addition

Hydrogen addition is one of the effective ways to reduce ignition delay. It improves the engine efficiency [19], however too much hydrogen addition will contribute to engine knocking. Szwaja and Grab-Logarinski [20] studied hydrogen addition with diesel in a CI engine, reporting that the energy ratio between hydrogen and diesel should not be more than 15% to avoid severe knock. This practice was followed in this study, while the n-heptane mass fraction was kept constant across all ranges to comply with further recommendations [20]. With the code validated in the previous sections, new results are presented for simulating diesel with hydrogen addition in an HCCI engine. It can be seen (Fig. 4) that the hydrogen addition helps reduce the ignition delay: the auto-ignition point is advanced significantly even though only a small amount of hydrogen is added (about 1%). If the hydrogen content is more than 20%, the mixture becomes rich and in this case, the n-heptane concentration has to be reduced to avoid rich mixtures. It seems that the hydrogen addition is able to increase the engine performance, however too much hydrogen addition will create knocking issues. These conclusions are to be validated against experiment in future work.

4. Conclusion

This paper has discussed the combustion behaviour of diesel HCCI engines for different operating conditions. Once the intake temperature is increased above a certain threshold, the in-cylinder peak pressure will decrease with increasing intake temperature. However, the in-cylinder peak pressure increases with increasing equivalence ratio over the range studied, so attempting to control the engine by this mechanism is not a good option as it will create knocking. Increasing the hydrogen content will also increase the in-cylinder peak pressure; therefore the hydrogen content should be no more than 20%. It was found that the combustion phasing is advanced by increasing all the parameters (intake temperature, equivalence ratio, and energy ratio), and therefore the auto-ignition can be controlled. Future work is needed to investigate all these factors on HCCI engines' performance.

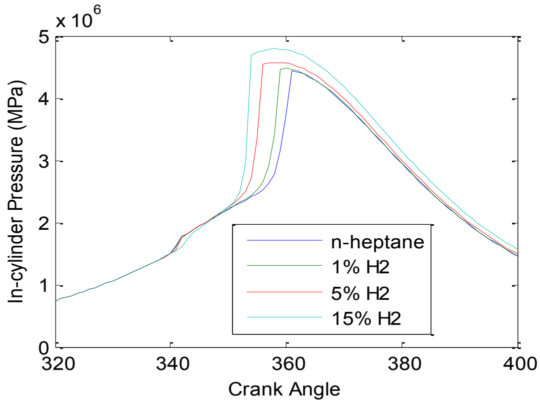

Figure 4 Predicted effect of hydrogen addition on the in-cylinder pressure for fixed n-heptane injection: CR=10.0, N=900 rpm, T_{in}=40°C, P_{in}=95 kPa

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