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Academic @ Paper
ISSN 2146-9067
International Journal of Automotive Engineering and Technologies
Vol. 4, Issue 1, pp. 54 – 62, 2015

International Journal of Automotive Engineering and Technologies
http://www.academicpaper.org/index.php/IJAET

Original Research Article

Thermo-kinetic modelling of variable valve timing effects on HCCI engine combustion

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Abstract

In this study the effects of variable valve timing on the combustion of a Homogeneous Charge Compression Ignition (HCCI) engine have been analysed using a new modelling approach for HCCI engine cycle. A novel sequential modelling platform is developed using a combination of detailed multi-zone thermo-kinetic combustion model, 1D intake flow model and exhaust gas flow model. The new model utilizes CHEMKIN-PRO and GT-POWER software along with in-house exhaust gas flow model. Experimental data from a single-cylinder HCCI engine is used to validate the model. Validation results show that the model can predict combustion phasing and Indicated Mean Effective Pressure (IMEP) with average errors of 1.1 crank angle degrees (CAD) and 0.3 bar, respectively. The experimentally validated model is then used to investigate the effects of intake valve timing on HCCI auto-ignition radicals, zonal temperature, combustion phasing, IMEP, and exhaust emissions.

Keywords: Homogeneous Charge Compression Ignition (HCCI), Sequential Model, Multi-Zone, Variable Valve Timing (VVT)

1. Introduction

HCCI which stands for Homogeneous Charge Compression Ignition is an advanced combustion mode that holds the promise of lowering emissions and increasing fuel economy in Internal Combustion (IC) engines 1,2. Combustion control is one major challenge to the market penetration of HCCI technology 1,3. HCCI combustion is primarily controlled by thermo-kinetic reactions, while turbulence/mixing are found to be of a lower influence as compared to the kinetic effects 1,3-5. In order to achieve HCCI combustion in conventional IC engines, the specific energy of the charge entering the cylinder needs to be increased to achieve auto-ignition 3. Several methods can be found in the literature to enable HCCI combustion 6. Intake air heating, high boost pressure, high compression ratio, dilution by hot external Exhaust Gas Recirculation (EGR) and VVT are some of the ways found in literature. It is the conditions at Intake Valve Closing (IVC) which affect the control and the performance of an HCCI engine and changing the valve timing events affect the temperature, pressure and mixture composition at IVC 4. For a fully flexible variable valve actuation system the parameters of lift, duration and timing can be changed independent of each other 7. In a simpler approach, only the valve timings can be varied, keeping the lift and the duration same.

Figure 1 describes three methods associated with valving strategies that have been used for HCCI combustion. The first two methods, including Recompression and Rebreathing, use the effect of internal EGR while the third

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Note: This paper has been presented at the International Conference on Advanced Technology & Sciences (ICAT'14) held in Antalya (Turkey).

method is used for changing the effective Compression Ratio (CR) by advancing or retarding the IVC. A special case of Miller Cycle analysis can be done by changing IVC timing so as to have a longer expansion stroke as compared to the compression stroke 8.

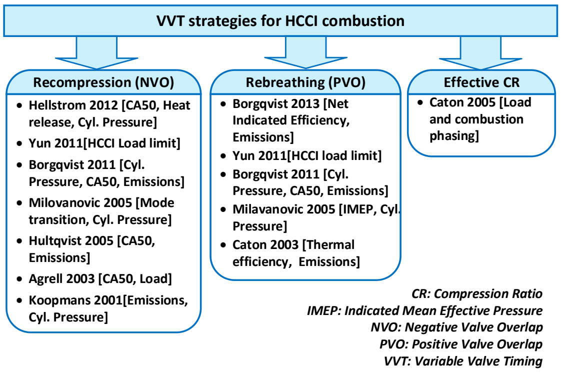

Figure 1.Background of main VVT strategies for HCCI combustion.

Recompression consists of trapping exhaust gases by not letting them out from the cylinder in the exhaust stroke 3,9-13. Rebreathing 4,14,15 is achieved by the use of positive valve overlap (PVO) where both intake and exhaust valves are kept open over the gas exchange Top Dead Center (TDC). This enables the expelled exhaust gases to be sucked in along with fresh charge during the intake stroke 14. Caton et.al 8 studied the effects of changing the effective CR on an HCCI engine for independent load and combustion phasing. The amount of dilution was fixed, and it was found that the IVC timing played a significant role in controlling HCCI combustion. A similar study in 10 concluded that the method of IVC timing control can be successfully used to extend the range of HCCI operation, since the amount of Negative Valve Overlap (NVO) achievable in the Recompression method is limited by the engine valve train system.

The advancement of numerical models for simulating combustion of HCCI engines has required the improvement of detailed thermo-kinetic models to understand HCCI combustion as a function of engine control variables. Computational models have expressed the importance of considering this fact that in-cylinder mixture is in-homogeneous, specifically with respect to temperature. This in-homogeneity is caused by mixing and heat transfer from the combustion chamber walls. The level of temperature stratification determines the rate of heat release and the tendency to knock 3,16. This restricts the analysis to model in-cylinder mixtures as a single zone and requires applying 3-D Computational Fluid Dynamics (CFD) code.

This study will focus on the thermo-kinetic modelling process for HCCI combustion to investigate VVT effects. Since CFD approach is time consuming, in this study a sequential thermo-kinetic modelling platform is developed using software packages of CHEMKIN-PRO and GT-POWER along with an exhaust stroke gas flow model 17. The new model is a substitute for the time consuming and computationally intensive CFD modelling. The combustion modelling done in this way yields results comparable with experimental data and in a short time. This work focuses on simulating the effects of IVC timing on HCCI combustion, but the modelling platform is comprehensive and can be used to simulate the impacts of other VVT strategies on HCCI combustion.

The contribution from this work is developing a modelling approach to predict and understand VVT impacts on HCCI combustion. The time required for obtaining results is short as compared to other sequential modelling approaches 16,18 which involve CFD. This paper is presented as follows. Section II describes the developed model for HCCI combustion. Section III describes engine specifications, model validation and core combustion analysis along with the simulation results. Summary and conclusions are presented in section IV.

2. Model Description

A full-cycle computationally-efficient HCCI model is developed to predict valve timing effects on combustion and performance metrics of an HCCI engine. The model consists of three components including (i) intake flow model to predict

IVC temperature and pressure, (ii) CHEMKIN-PRO multi-zone thermo-kinetic model to predict combustion metrics, and (iii) exhaust stroke gas flow model during exhaust stroke to complete simulation of the whole HCCI cycle for predicting IMEP. An overview of model components along with valve timing events is shown in Figure 2(a).

2.1. Intake flow model

The process from Intake Valve Opening (IVO) to IVC is modelled according to the 1-D flow simulation model using GT-POWER. The conditions at IVC influence subsequent combustion parameters and hence the engine output. Thus, it is necessary to calculate the IVC parameters considering flow through valves. Since it is difficult to measure the values at IVC crank angle experimentally, these values are obtained by building the same engine model in GT-POWER. The GT-POWER model provides in-cylinder temperature and pressure values at IVC crank angle.

2.2. Thermo-kinetic combustion model

A multi-zone combustion model is designed with the assumption that the mixture properties at IVC are uniform. The cylinder volume is divided into number of imaginary zones with respect to in-cylinder temperature distribution. Multi-zone modelling is carried out using CHEMKIN-PRO for simulating the HCCI engine combustion. Later, in order to see the effect of VVT on the in-cylinder pressure trace, the IVC timings are changed in GT-POWER and the pressure and temperature values at IVC are given as input to CHEMKIN-PRO. An overview of the process used to carry-out combustion simulations and validate the model with experimental data 19 is shown in Figure 2(b).

Combustion simulation includes closed engine cycle which begins from IVC and ends at Exhaust Valve Opening (EVO). The combustion chamber is divided into ten zones (Figure 3) using the results from previous HCCI studies 16,20. Combustion takes place within the hottest zone and then extends to the surrounding zones. Since HCCI combustion occurs rapidly, mass and heat transfer between zones can be neglected in the multi-zone model 16. Thus, the zones interact just by compressing each other.

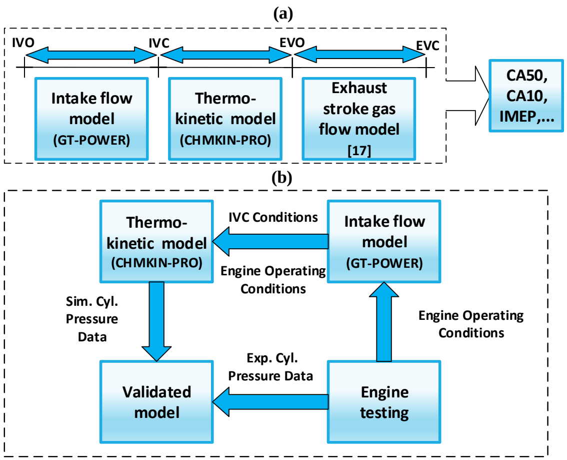

Figure 2. (a): Sequential modelling platform to simulate full HCCI engine cycle (IVO/C and EVO/C stand for Intake Valve Opening/Closing and Exhaust Valve Opening/Closing, respectively.), (b): Process used to experimentally validate HCCI thermo-kinetic combustion model.

With the absence of flame propagation, the HCCI combustion process is controlled by chemical kinetics. The Lawrence Livermore detailed chemical mechanism 21 for n-heptane is used in this study. This mechanism consists of 2827 reactions and more than 500 species and has been successfully validated for HCCI combustion.

Woshni heat transfer correlation 22 is used to model the heat transfer through the cylinder walls. The heat transfer correlation based on in-cylinder conditions is given below:

$$h_{wall} = \alpha_{scaling} B^{-0.2} P^{0.8} T^{-0.53} \omega^{0.8} \quad (1)$$

where, B is the cylinder bore (cm), P is the instantaneous in-cylinder pressure (kPa) and T is the mixture temperature (K). An appropriate value of $\alpha_{scaling}$ is selected to adopt this correlation for the engine geometry in this study. The rate of change of the mixture temperature is obtained by following equation 22:

$$\frac{dT}{dt} = \frac{\frac{-Pdv}{dt} - \frac{dQ_w}{dt} - \sum_i \frac{dN_i}{dt} \bar{h}_i + R_u T \sum_i \frac{dN_i}{dt}}{\sum_i N_i \bar{C}_{p,i} - N_{mix} R_u} \quad (2)$$

where, P is the in-cylinder gas pressure, N_i and $\bar{C}_{p,i}$ are the number of moles and the molar specific heat of the i_{th} species. R_u is the universal gas constant and V is the cylinder volume which is calculated at every crank angle from engine geometry.

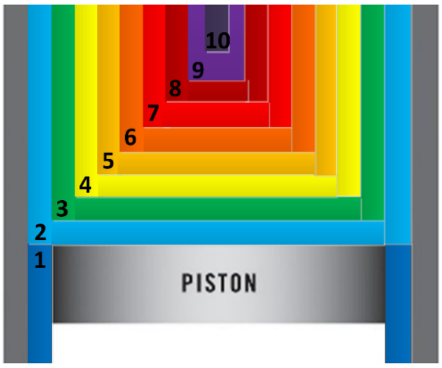

Figure 3. Configuration of the zones in the HCCI thermo-kinetic model.

Details of multi-zone thermo-kinetic modelling of HCCI can be found in 16. The main outputs of the combustion model include in-cylinder pressure trace from IVC to EVO, zonal temperature, combustion phasing, and engine-out emissions. These outputs will be used later to analyze HCCI combustion as a function of IVC variations.

2.3. Exhaust stroke gas flow model

The combined intake flow model and the thermo-kinetic model simulate the in-cylinder pressure from IVO to EVO. But in-cylinder pressure during the whole engine cycle is required in order to calculate the IMEP. Thus an exhaust stroke gas flow model from 17 is used to simulate the in-cylinder pressure from EVO to Exhaust Valve Closing (EVC). This model determines dynamics of the gas flow across the exhaust valves by using one dimensional, compressible and isentropic orifice flow 17. The model also calculates mass fraction and temperature of residual gases which are key control parameters for VVT strategies in HCCI engines.

3. Results and Discussion

3.1. Engine specifications

The experimental data is taken from 19 for a Ricardo Mark III single cylinder engine which has two camshafts actuating four valves. The engine specifications are listed in Table 1. The valve timing diagram and intake valve phasing are shown in Figure 4 and Figure 5, respectively.

Table 1. Engine specifications.

Parameter	Value
Bore × Stroke (mm)	80 × 88.9
Compression Ratio	10:1
Displacement Volume (L)	0.447
IVO/IVC (° aBDC)	-175/+55
EVO/EVC (° aBDC)	-70/-175

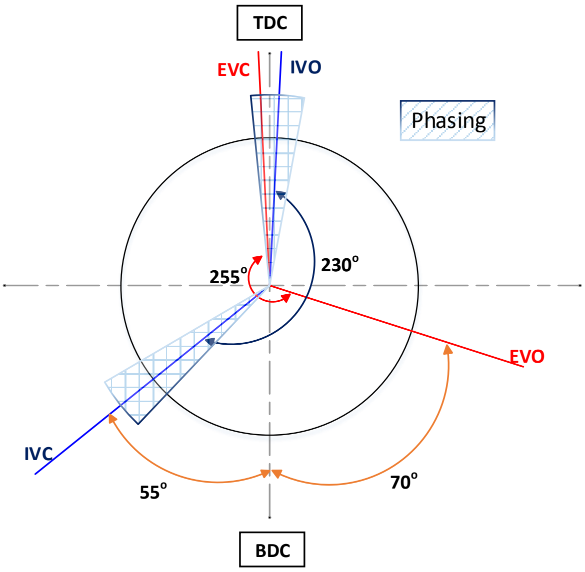

Figure 4. Valve timing diagram for Ricardo engine including phasing done in this study.

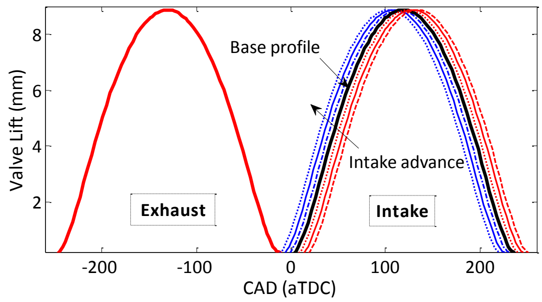

Figure 5. Valve profiles studied in this work (intake valves phased).

3.2. Model validation

Figure 6 shows the comparison of simulated and experimental in-cylinder pressure traces for three different HCCI operating conditions with n-heptane fuel. The comparison results show a good agreement between simulations (Sim.) and experiments (Exp.). The experimental and simulation values for CA50 and IMEP are compared in Table 2. Average errors for predicting CA50 and IMEP are 1.1 CAD and 0.3 bar, respectively. Thus the developed model is accurate for prediting the combustion phasing (CA50) and load (IMEP) for the HCCI engine.

3.3. Combustion analysis

Auto-ignition of hydrocarbon fuels like n-heptane is initiated by the following chemical reaction 3:

$$H_2O_2 \rightarrow OH + OH \qquad (3)$$

This reaction is temperature dependant and needs temperatures of around 1000K for hydrogen peroxide (H_2O_2) decomposition. The hydroxyl (OH) and H_2O_2 are the major chemical radicals to trigger the auto-ignition in HCCI. The concentrations of OH and H_2O_2 as a function of crank angle are presented in Figure 7. Concentration of H_2O_2 increases as the cycle proceeds and reaches its peak value close to the main combustion event.

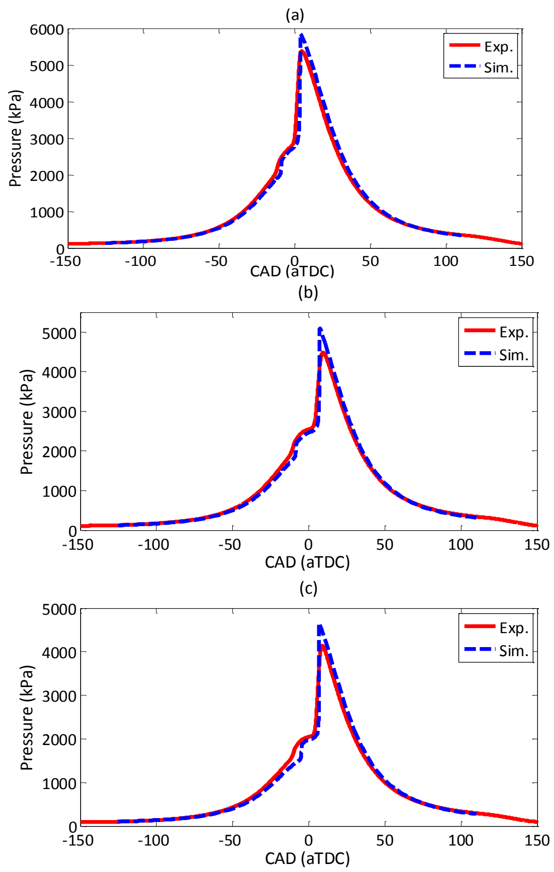

Figure 6. Comparison between experimental (Exp.) and simulated (Sim.) in-cylinder pressure traces.
(a) n-heptane, RPM= 1016, ϕ= 0.45, T_{man}= 87.6 °C, P_{man}= 117.2 kPa;
(b) n-heptane, RPM= 1016, ϕ= 0.45, T_{man}= 87.6 °C, P_{man}= 108.8 kPa;
(c) n-heptane, RPM= 920, ϕ= 0.56, T_{man}= 90.8 °C, P_{man} =89.1 kPa.

Subsequently, due to H_2O_2 decomposition the concentration of OH radicals increases spontaneously near the main combustion point. A pool of radicals is then formed which follow chain branching and propagation reactions, leading to very fast combustion close to an ideal constant volume combustion in the ideal Otto cycle.

Table 2**.** Comparison of experimental and simulation results for CA50 and IMEP for the operating conditions in Figure 6.

	CA50 (CAD aTDC)		IMEP (bar)	
	Sim.	**Exp.**	**Sim.**	**Exp.**
a	3.4	1.7	5.4	5.1
b	7.0	6.2	4.9	4.7
c	6.8	6.1	4.7	4.3

The zonal temperatures are shown in Figure 8. The core zone #10 has the highest temperature; thus, H_2O_2 decomposition begins from this zone, followed by the neighbouring zone #9. Simulated temperature results show the lowest gas temperatures for the zones 1 and 2. These two zones represent crevices and wall boundaries where majority of the unburned Hydrocarbon (uHC) and Carbon Monoxide (CO) emissions occur.

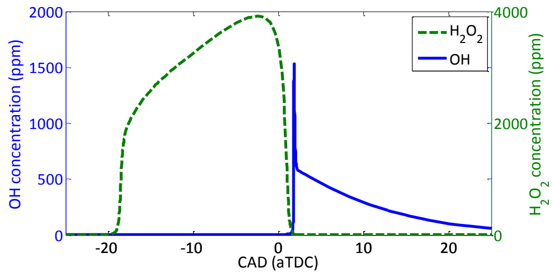

Figure 7. Concentration of OH and H_2O_2 radicals for zone #10 for case (a) from Fig. 6.

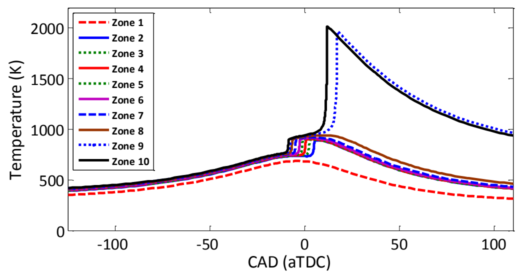

Figure 8. Zone temperature distribution for the case (a) from Figure 6.

3.4. Effect of IVC on HCCI combustion

The case (a) from Figure 6 with IVC= -125 °aTDC and the intake pressure of 117.2 kPa is selected as a baseline to investigate the impacts of valve timing on HCCI combustion. The simulation results are presented in Figure 9 – Figure 13 to show the impact of IVC timings on the in-cylinder pressure, temperature, IMEP, combustion phasing, Burn Duration (BD), and engine-out uHC and CO emissions at EVO. It can be seen that as the IVC is advanced from -125°aTDC to -140°aTDC, the peak in-cylinder pressure increases from 58.5 bar to 61.2 bar (Figure 9), peak in-cylinder temperature increases from 2067 K to 2074 K (Figure 10), and the CA50 advances from 3.4° to 2.2° aTDC (Figure 11). While retarding the IVC from base position to -110°aTDC causes the peak in-cylinder pressure to reduce from 58.5 bar to 41.3 bar, peak in-cylinder temperature reduced from 2067 K to 1967 K and the CA50 retarded from 3.4° to 16.2°. It can also be seen that, the percentage change in all the results is more for the retarding phase compared to those in the advancing phase.

The difference in the percentage change during advancing and retarding IVC shows how close the stable operating limits are. The HCCI engine operation is limited by the knock limit through advancing IVC and is limited by the misfire limit through retarding IVC. Changing the IVC timing affects the temperature profile of the hottest zone #10; thus, advancing IVC causes temperature of the zone #10 to increase at a faster rate than before, leading to an earlier auto-ignition. This is why the crank angle for 10 percent burnt fuel (CA10) and the crank angle for 50 percent burnt fuel (CA50) advances and BD reduces. Reduction in BD is associated with higher peak in-cylinder pressure rise rate during the main combustion as seen in Figure 9 and Figure 11. Closing the intake valve early causes to lose the inertia effect of incoming charge. But because of low operating speeds (1016 rpm), the advantage lost is expected to be small. The IMEP is seen to drop as the IVC is retarded. This suggests a decrease in engine load because of low effective compression ratios and also because of charge rejection into the intake manifold.
From Figure 12 it is seen that, the concentrations of uHC and CO increase as the IVC is delayed. The reason for this can be attributed to the fact that the charge has a difficulty in auto-igniting due to the low effective CR. These cases with low effective CR have lower average zonal temperatures. Hence, the fuel trapped in these zones does not combust or partially combusts. In addition, the uHC production is mainly associated with the zones 1 and 2, and as the average zone temperature in these zones increases the uHC concentration is seen to reduce (Figure 13). The reason is that, in the cases with higher average temperatures for zones 1 and 2, some amount of fuel in zone 2 reaches an appropriate temperature and combusts, hence less uHC concentration is observed in these cases.

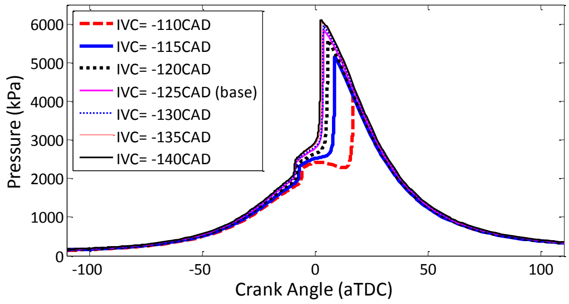

Figure 9. In-cylinder pressure as a function of IVC timing.

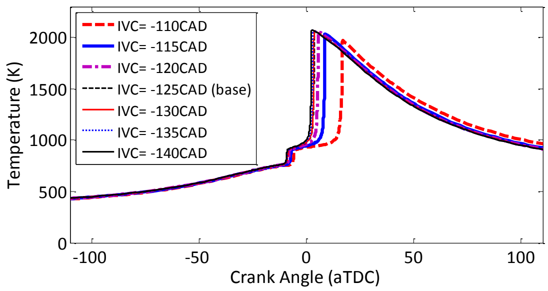

Figure 10. In-cylinder gas temperature as a function of IVC timing.

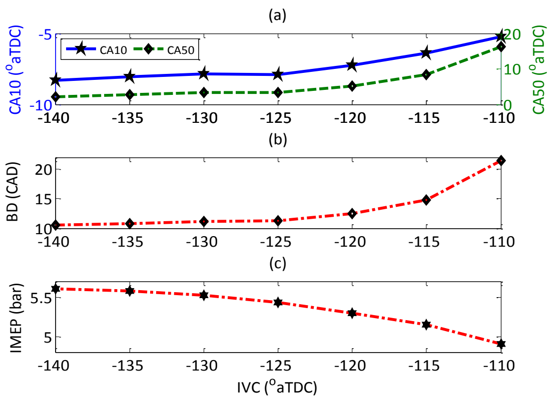

Figure 11. CA10, CA50, burn duration and IMEP as a function of IVC timing.

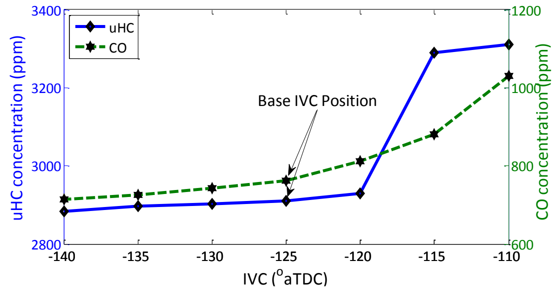

Figure 12. Engine-out Concentration of uHC and CO as a function of IVC timing.

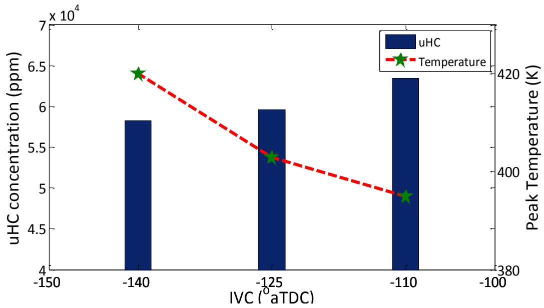

Figure 13. uHC concentration and peak temperature for zones 1 and 2 as a function of IVC timing. The values in this figure are averaged for the zones 1 and 2.

From figure 12 it is seen that, the concentrations of uHC and CO increase as the IVC is delayed. The reason for this can be attributed to the fact that the charge has a difficulty in auto-igniting due to the low effective CR. These cases with low effective CR have lower average zonal temperatures. Hence, the fuel trapped in these zones does not combust or partially combusts. In addition, the uHC production is mainly associated with the zones 1 and 2, and as the average zone temperature in these zones increases the uHC concentration is seen to reduce (Figure 13). The reason is that, in the cases with higher average temperatures for zones 1 and 2, some amount of fuel in zone 2 reaches an appropriate temperature and combusts, hence less uHC concentration is observed in these cases.

4. Conclusion

A new sequential modelling approach was developed to study the effects of valve timing on HCCI engine cycle. The new model captures HCCI thermo-kinetic reactions through a detailed multi-zone combustion model developed in CHEMKIN-PRO. 1D intake and exhaust gas flow models were linked to the combustion model to (i) incorporate intake valve timing effects on the engine closed cycle (IVC-EVO), and (ii) simulate the full engine cycle for predicting engine performance metrics including IMEP. The combined model was validated with the experimental data collected from a single-cylinder HCCI engine with n-heptane fuel. The combustion model, which includes 2827 reactions with over 500 species, could predict HCCI combustion phasing with a maximum error of 1.7 CAD. In addition, the full-cycle engine model could predict IMEP with a maximum error of 0.4 bar.

The IVC timing was varied for 30 CAD and its impact was studied on HCCI in-cylinder pressure trace, combustion phasing (CA10, CA50, BD), major auto-ignition radicals (OH and H_2O_2), zonal temperature distributions, and engine-out emissions (uHC, CO). IVC timing impacts on auto-ignition (CA10) and peak in-cylinder temperature were linked to the core combustion zone, while engine-out emissions were linked to the zones 1 and 2 with the peak temperature less than 450K. Advancing IVC led to early combustion phasing, higher IMEP, and lower uHC and CO engine-out emissions. But this also leads to the higher peak in-cylinder pressure and higher pressure rise rate that will restrict HCCI operation by the knock limit. The developed model was found to be an effective simulation platform to characterize valve timing impacts on HCCI combustion. The developed model is comprehensive and has the capability to study effects of other HCCI engine control variables including exhaust valve timing, boost pressure, and intake temperature due to the flexibility offered by the intake and exhaust gas flow models.

Acknowledgment

The authors acknowledge Prof. C. R. Koch from the University of Alberta for providing the experimental data 19 which was used to validate the combustion model in this work.

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