Evaluating the EGR-AFR Operating Range of a HCCI Engine

Amit Bhave, Markus Kraft
Department of Chemical Engineering, University of Cambridge
Fabian Mauss
Division of Combustion Physics, Lund Institute of Technology
Aaron Oakley, Hua Zhao
Department of Mechanical Engineering, Brunel University

ABSTRACT

We present a computational tool to develop an exhaust gas recirculation (EGR) – air-fuel ratio (AFR) operating range for homogeneous charge compression ignition (HCCI) engines. A single cylinder Ricardo E-6 engine running in HCCI mode, with external EGR is simulated using an improved probability density function (PDF) based engine cycle model. For a base case, the in-cylinder temperature and unburned hydrocarbon emissions predicted by the model show a satisfactory agreement with measurements [Oakley et al., SAE Paper 2001-01-3606]. Furthermore, the model is applied to develop the operating range for various combustion parameters, emissions and engine parameters with respect to the air-fuel ratio and the amount of EGR used. The model predictions agree reasonably well with the experimental results for various parameters over the entire EGR-AFR operating range thus proving the robustness of the PDF based model. The boundaries of the operating range namely, knocking, partial burn, and misfire are reliably predicted by the model. In particular, the model provides a useful insight into the misfire phenomenon by depicting the cyclic variation in the ignition timing and the in-cylinder temperature profiles. Finally, we investigate two control options, namely heating intake charge and trapping residual burned fraction by negative valve overlap. The effect of these two methods on HCCI combustion and CO, HC and NO\textsubscript{x} emissions is studied.

INTRODUCTION

Homogeneous Charge Compression Ignition (HCCI), an advanced mode of engine operation is attractive on account of its efficiency as high as the conventional modes of internal combustion engine operation, low NO\textsubscript{x} emissions, and virtually no particulate matter (PM) emissions. Commercializing HCCI technology, however, remains a formidable challenge due to its narrow operating regime and intrinsic difficulties in controlling auto-ignition timing.

An operating range describes the limits of a stable engine operation for a range of operating conditions, and has been expressed in the literature in as load-speed operating windows and 2-D maps as a function of EGR and AFR. Early use of operating maps for HCCI was presented in ref. [1]. In that study the operating regime of a single cylinder four-stroke HCCI engine was mapped as a function of equivalence ratio (1/AFR) and EGR rates. Drawbacks of HCCI in terms of a small operating window and difficulty in controlling the auto-ignition were pointed out. Later, a homogeneous reactor model has been used to map the operation of a methane fuelled HCCI engine [2]. The region of acceptable HCCI operation was depicted by plotting various parameters such as indicated efficiency, burn duration, NO emissions and ignition timing with respect to the residual burned fractions and AFRs. The limits of the maps were given by partial burn, region of fast combustion, and a region of early combustion. The transition between partial burn and complete burn was found to be extremely sharp. In case of two-stroke HCCI operation, a load-speed operating window was plotted while demonstrating direct high pressure liquid injection HCCI operation for the first time [3]. On comparing the operating fields for three injection methods, namely: direct high pressure liquid injection, indirect (premixed) injection and air-assisted injection, the first method was found to exhibit the widest operating range. Taking a similar approach to the work in ref. [1], the operating range of HCCI engine with regard to AFR and EGR has been established, and a range of stable HCCI operation was identified for various fuels such as alcohols, and blends of gasoline, while maintaining constant inlet temperature and compression ratio. A large difference in the tolerance to dilution existed between the various fuels studied [4]. The feasible range of a naturally aspirated HCCI engine operation has been scanned by using three valve timing events to cover the complete
range of the unthrottled HCCI engine [5]. Three zones that limit the stable HCCI operation were identified on a load-speed map. Zone 1 given by high cycle to cycle variation at low-load and low-speed, zone 2 representing knocking and zone 3 with high speeds and low loads giving misfire. In another study, a four-stroke multi-cylinder engine was operated in HCCI mode with a stoichiometric AFR without intake charge heating or higher compression ratios, by trapping large amount of residual burned gases [6]. The load-speed operating map showed a stable HCCI operation between load range, 0.5 to 4 brake mean effective pressure (BMEP) and speed range 1000 to 3500 RPM. In the load-speed range investigated, knocking was not observed but the two main limits of the stable operation were identified. For high loads, at each speed, maximizing the airflow resulted in maximum possible BMEP. At each load there was a minimum BMEP which was limited by misfire. In particular for miniature HCCI engines, operational maps have been presented using a homogeneous modelling approach [7]. Based on the mappings, it was pointed out that the extent of the engine operational space can be increased at the expense of a reduction in power density. Lately, load-speed operating maps have been developed to demonstrate a stable HCCI combustion initiation in a five-cylinder engine with variable compression ratio and inlet air heating via exhaust heat recovery [8].

Computational modelling provides a time- and cost-effective mean to develop such operating ranges and evaluate strategies to expand them. Recently, a homogeneous reactor model (a perfectly stirred reactor) based engine cycle simulator was implemented to predict load-speed performance maps for HCCI engines [9]. In that study the operating limit at higher loads, i.e. knock, was investigated in detail by introducing a dimensionless knock parameter. Probability density function (PDF) based [10] closed volume [11,12] as well as engine cycle [13,14] models have been successfully applied for modelling HCCI operation. These models include detailed chemical kinetics and do not face reaction rate closure problems. Furthermore, the models account for turbulent mixing, fluid-wall interactions and fluctuations, inherent to an engine operation. Thus unlike the homogeneous reactor models, in addition to developing an operating window for various combustion and engine parameters, the PDF models can be utilized to predict operating maps for detailed emissions studies.

In this paper, the PDF based engine cycle model as explained in ref. [13] has been applied to develop an EGR-AFR operating range for various combustion parameters, emissions, and engine parameters. In addition to the narrow operating window, challenges in controlling HCCI operation need to be overcome. In the second part of the paper, two distinct approaches adopted to overcome the HCCI control hurdle are investigated:

1) Increasing the inlet charge temperature by incorporating a heater in the engine cycle.

2) Trapping of residual burned fraction using variable valve actuation with standard compression ratios.

**ENGINE DESCRIPTION**

In this section, the geometry and the operating parameters of the Ricardo E-6 engine (Figure 1) are discussed. This is followed by the description of the experimental procedures adopted for the measurements and construction of the operating window. This explanation is included here to complement the simulation procedure explained in the next section. All the experimental results were taken from ref [4].

![Ricardo E-6 engine run in HCCI mode.](image)

The specifications of the four-stroke Ricardo engine are given in Table 1. The compression ratio for the engine was variable in the range 4.5:1 to 18:1 using a worm gear, able to control the height of cylinder head relative to the crankshaft. It was measured with a calibrated micrometer mounted at the side of the cylinder and was fixed at 11.5:1 for the present study. The valve timings given in Table 1 yielded a valve overlap period of around 14° around TDC on the induction stroke and prevented excessive exhaust back-flow when the intake manifold pressure is low relative to the exhaust. The engine was fuelled with PRF-95, i.e., a mixture of 95% iso-octane and 5% n-heptane, by volume.
**Table 1:** Ricardo E-6 engine geometry and operating parameters.

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displaced volume</td>
<td>504 cm³</td>
</tr>
<tr>
<td>Bore</td>
<td>76.2 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>111.1 mm</td>
</tr>
<tr>
<td>Exhaust valve open</td>
<td>43° BBDC (at 5 mm lift)</td>
</tr>
<tr>
<td>Exhaust valve close</td>
<td>6° ATDC (at 5 mm lift)</td>
</tr>
<tr>
<td>Inlet valve open</td>
<td>8° BTDC (at 5 mm lift)</td>
</tr>
<tr>
<td>Inlet valve close</td>
<td>36° ABDC (at 5 mm lift)</td>
</tr>
<tr>
<td>Speed</td>
<td>1500 rpm</td>
</tr>
<tr>
<td>Fuel</td>
<td>PRF-95</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>11.5</td>
</tr>
</tbody>
</table>

**EXPERIMENTAL SET-UP**

The experimental set-up is shown in Figure 2, where d and L denote the internal diameter and the length of a pipe and r denotes the radius of a bend. Air was mixed with the EGR (when the EGR valve was open), and passed through a 3 kW intake gas heater. The heated gas was then passed through the manually controlled throttle. A port fuel injector directed towards the intake valve was mounted. The exhaust gases were split into two streams.

The main stream passed through the gate valve used to control the exhaust back-pressure, to the exhaust measurement unit. The second stream passed through the EGR valve and mixed with the fresh air stream to form an almost homogeneous air-EGR mixture. A water-cooled piezoelectric type pressure transducer, capable of measuring gauge pressures in the range 0-100 bar was used in the engine block. For the measurement and control of the intake and exhaust gas temperatures as well as the coolant and oil temperatures, thermocouples were employed at various locations around the engine. A non-dispersive infrared absorption cell was employed to measure CO, CO₂ and O₂. The NOₓ emissions were analyzed using a chemiluminescent NOₓ analyzer. The exhaust unburned hydrocarbon concentrations were measured using the flame ionization detection technique.

**NUMERICAL MODEL**

In this section, the numerical model implemented as well as the comparison between model calculations and experiments for a base case are discussed.

**MODEL DESCRIPTION**

An improved PDF based full cycle model was employed to simulate the combustion, emissions and the gas exchange processes in the HCCI engine. The integrated model comprises of the PDF based stochastic reactor model coupled with a 1-D engine cycle simulator, GT-POWER. The model has been explained in detail in the previous work [13].

The engine mapped on the 1-D code interface is shown in Figure 3. For the present engine with EGR, 49 uncoupled cycles (1-D code only) were found to be necessary to stabilize the mass flow rates on the basis of the flow through the EGR valve. This was followed by

![Figure 2: Experimental set-up](image-url)

![Figure 3: Engine set-up map on the 1-D code interface](image-url)
4 homogeneous reactor model based coupled cycles and 2 PDF model based coupled cycles. The first PDF based coupled cycle was performed with 50 stochastic particles and the second with 100 particles. The total computational time for one complete simulation with 55 cycles was 17 h on a Athlon XP2000, 1.67 GHz PC. While providing the temperature at IVC, the 1-D code accounts for the residual burned fraction, EGR and fresh charge. This temperature was assigned to all the stochastic particles as the initial condition. Similarly, the composition of each stochastic particle in the ensemble is same at IVC. The chemical mechanism for the primary reference fuel containing 157 species and 1552 chemical reactions, as explained in ref. [13] was used. The stochastic mixing model by Curl is used to account for the effect of turbulent mixing. In that, two distinct stochastic particles are chosen from the ensemble according to uniform distribution and are mixed depending on the characteristic time, \( \tau \), for mixing [13].

The sub-model for convective heat loss is based on Woschni’s heat transfer coefficient. The model parameter \( C_h \) is related to the temperature fluctuation \( h_i \) as,

\[
    h_i = \frac{T_i - T_w}{C_h}
\]

where \( T_i \) is the temperature of the \( i \)th particle and \( T_w \) stands for the wall temperature. The sub-model has been explained in detail previously [13].

MODEL VALIDATION

Before constructing the EGR-AFR operating range for the present engine, the model was calibrated by comparing the in-cylinder temperature and emissions with the measurements for a base case. The engine operating conditions are as given in Table 1 and the model parameters are given in Table 2.

Table 2: Model parameters.

<table>
<thead>
<tr>
<th>Variables</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_w )</td>
<td>450 K</td>
</tr>
<tr>
<td>( T_{IVC} )</td>
<td>493 K</td>
</tr>
<tr>
<td>( C_h )</td>
<td>40.0</td>
</tr>
<tr>
<td>Fuel mass</td>
<td>7.5 mg/cycle</td>
</tr>
<tr>
<td>( \tau )</td>
<td>0.02 s</td>
</tr>
</tbody>
</table>

For these conditions the in-cylinder temperature profile and the unburned HC emissions predicted by the model were compared with the experimental results as shown in Figure 4. The comparison showed a reasonably good agreement for the in-cylinder temperature profile. The auto-ignition timing and the peak temperature were predicted well, however the temperature at auto-ignition was over-predicted as compared to that in the measurements. The comparison of the experimental and predicted values of HC emissions suggested a reliable HC prediction. Having validated the model, the parameters namely, \( T_w \), \( C_h \) and \( \tau \) used in Table 2 were kept constant throughout the present paper. The model was then applied to map the operating window for the HCCI engine as described in the next section.

EGR-AFR OPERATING RANGE

In the present paper, the integrated full cycle model was run for 23 points (each point corresponding to a specific air-fuel ratio and EGR) as shown in Figure 5. The total computational time for these 23 points was around 14 days on an Athlon XP2000, 1.67 GHz PC. Interpolation was used to develop the contour plots for various parameters such as indicated mean effective pressure (IMEP), combustion duration, temperature at IVC, indicated thermal efficiency as well as the CO, HC, and NOx emissions with respect to the AFR and the amount of EGR. The contour plots for the predicted quantities were compared with measurements. Thus, such a comparison over the entire EGR-AFR operating range of the engine provided a rigorous validation of the model calculations. The solid lines in Figure 5 were established by the engine mapping process in ref. [4].
The EGR-AFR operating range depicted in Figure 5 is bounded by three regions, namely: partial burn, misfire, and knock. Knock occurs when an excessively violent rise in heat release causes pressure fluctuations. Partial burn occurs when the air-fuel ratio is too lean to allow the full oxidation of the fuel. Misfire is caused due to an intolerable amount of exhaust gases being recycled back into the cylinder, causing some of the engine cycles to fail to ignite. The cycle-to-cycle variation due to this effect is further aggravated by the lean air-fuel ratios. In the experiments, the misfire condition was quantified as the point at which more than 1% of the cycles failed to burn. The base case used for validation in the previous section is denoted by the cross at a point corresponding to $\lambda = 2.5$ and 32% EGR.

Figures 6 to 23 depict the comparison of the model predictions and measurements for various parameters over the entire operating range. The IMEP prediction (Figure 6) and the measurements (Figure 7) showed a good agreement. Higher loads were obtained nearer to the knock boundary, as the AFR becomes richer. The highest attainable load predicted by the model was 3.5 bar (93% of the experimental value). With increasing air dilution, low loads were achieved. At such low loads, partial burning set in with a loss in combustion efficiency and rise in fuel consumption. The model successfully predicted the partial burn boundary on the basis of two factors; very high CO and HC emissions, and near zero IMEP (for points lying in the partial burn region in Figure 5). The rate of in-cylinder pressure rise is an important parameter to identify the onset of knock. From Figure 8 and 9, it was observed that the isolines run parallel to the knock boundary. Thus the rate of pressure rise showed a qualitatively similar dependence on air and EGR dilution. For the points lying in the knock region of Figure 5, an excessively high rate of pressure rise was predicted. The value is approximately 20 bar/CAD and indicates onset of knock in agreement with the results elsewhere [15,16]. Alternative approaches to account for knock while modelling HCCI, include the modification of the convective heat transfer coefficient with an additional term for the rate of pressure rise [17] and the use of knock parameter dependent on the rate of chemical heat release and volumetric expansion at the speed of sound [9].

The temperature at IVC (Figure 11) and the exhaust gas temperature (Figure 13) were reported in °C for the experimental results [4]. To facilitate the comparison, the model predictions for these two parameters are also given in the same units. In the experimental set-up the temperature at IVC as shown in Figure 11 was maintained in the range of 200 °C to 220 °C over the operating range. In the model set-up, the heater temperature was adjusted such that the temperature was maintained in the experimental range as shown in Figure 10.

The model predictions (Figure 12) and the experimental results (Figure 13) for exhaust gas temperature denote the highest values as conditions approached stoichiometric AFR, and the lowest values with high air dilution. Over the entire operating range the exhaust gas temperature was predicted well.

Indicated thermal efficiency and indicated specific fuel consumption are generally used to express the efficiency of an engine. The former dimensionless parameter is preferred over the latter when comparing a range of fuels on the same engine. Figures 14 and 15 show the operating maps for indicated thermal efficiency obtained from both model predictions and measurements. Similar to the IMEP behaviour, the richer the air-fuel mixture, the greater is the efficiency. With air dilution, the efficiency is reduced. The maximum and minimum efficiency values were predicted reliably compared to those obtained from measurements.

Combustion duration is calculated as the CAD difference between 10% and 90% mass fraction burned. With a rapid rate of combustion near the knock boundary, the combustion duration was about 6 CAD. The combustion duration increased with high dilution rates for air as well as EGR as shown in Figures 16 and 17. The convergence of the predicted isolines occurred near the misfire boundary (Figure 18). The isolines observed in the measurements (Figure 17), however, converged more densely at the misfire boundary near the stoichiometric AFR. The uncertainty related to the experimental evaluation of the mass fraction burned and the averaging of combustion duration over the cycles are possible sources of this discrepancy.

The charts for CO, NO, and HC emissions are given in Figures 18 to 23. The CO emissions depicted in Figure 18, increased with increasing air dilution. Near the partial burn boundary, maximum CO emissions were observed due to the incomplete oxidation of the AFR. In this region the CO emissions were reliably predicted by the PDF-based full cycle model. At high loads, the CO emissions reduced with better oxidation of the air-fuel mixture.

The NO emissions as shown in Figure 20 were the highest in the high load limit, due to the higher in-cylinder temperatures. In the proximity of the partial burn boundary, with very low in-cylinder temperatures, the NO emissions were predicted much lower than those observed experimentally.

Maximum specific unburned hydrocarbon emissions (Figure 22) were obtained near the partial burn boundary where the air dilution was the highest. This is due to the low overall combustion temperatures preventing the complete oxidation in this region. Minimum HC emissions were observed with high load limits. The HC emissions in the proximity of partial burn region were predicted accurately by the model as compared to the measurements. However, in the high load region of the window the emissions were under-predicted by 50%.
Figure 6: Calculated IMEP (bar) as a function of $\lambda$ and EGR.

Figure 8: Calculated $dP/dCAD$ (bar/CAD) as a function of $\lambda$ and EGR.

Figure 10: Calculated intake temperature ($^\circ$C) as a function of $\lambda$ and EGR.

Figure 7: Measured IMEP (bar) as a function of $\lambda$ and EGR [4].

Figure 9: Measured $dP/dt$ (bar/CAD) as a function of $\lambda$ and EGR [4].

Figure 11: Measured intake temperature ($^\circ$C) as a function of $\lambda$ and EGR [4].
Figure 12: Calculated exhaust temperature (°C) as a function of $\lambda$ and EGR.

Figure 13: Measured exhaust temperature (°C) as a function of $\lambda$ and EGR [4].

Figure 14: Calculated indicated thermal efficiency as a function of $\lambda$ and EGR.

Figure 15: Measured indicated thermal efficiency as a function of $\lambda$ and EGR [4].

Figure 16: Calculated combustion duration (CAD) as a function of $\lambda$ and EGR.

Figure 17: Measured combustion duration (CAD) as a function of $\lambda$ and EGR [4].
Figure 18: Calculated CO emissions (g/kWh) as a function of $\lambda$ and EGR.

Figure 19: Measured CO emissions (g/kWh) as a function of $\lambda$ and EGR [4].

Figure 20: Calculated NO$_x$ emissions (g/kWh) as a function of $\lambda$ and EGR.

Figure 21: Measured NO$_x$ emissions (g/kWh) as a function of $\lambda$ and EGR [4].

Figure 22: Calculated HC emissions (g/kWh) as a function of $\lambda$ and EGR.

Figure 23: Measured HC emissions (g/kWh) as a function of $\lambda$ and EGR [4].
It should be noted that the wall temperature changes with varying in-cylinder temperature over the operating range. A fixed temperature, however, was used to simulate the engine over the entire operating range. Thus, the prediction could be improved by accounting for a better estimation of wall temperature distribution. In summary, the combustion parameters, emissions and the engine parameters are predicted well by the model over the entire operating range. In consequence, for developing an operating range for the HCCI engine, the SRM based engine cycle simulator offers a reliable and time- as well as cost- effective tool. Following the rigorous model validation and development of the EGR-AFR operating range of the engine, model prediction of the misfire phenomenon is presented in the next section.

MISFIRE PREDICTION

Misfire occurs due to intolerable amounts of EGR in the cylinder. The points corresponding to $\lambda = 3.0$, EGR = 52% and $\lambda = 3.7$, EGR = 50% (Figure 5) are located closest to the region bounded by misfire occurrence. For such points, the simulation set-up comprising $50 + 4 + 2$ cycles was observed to be insufficient to capture the effect of misfire. Hence, in addition to the 50 uncoupled and 4 coupled cycles with homogeneous reactor based model, 10 SRM-PI based coupled cycles were used. All the other parameters were left unchanged.

For example, during cycle 60, the inlet charge failed to burn, resulting in a misfire. For the subsequent cycle 61, although the temperature at IVC was 10 K lower than that for cycle 60 (Figure 26), with 50% EGR percentage being recycled back, the large amount of unburned fuel from the cycle 60 was introduced in the next cycle. This rich fuel burned instantaneously and vigorously resulting in a high peak temperature in cycle 61. The ignition crank angle degree was delayed for cycle 61 as the air-fuel charge failed to burn, whereas, the ignition was advanced for the subsequent cycle.
In-cylinder temperature variation at point, $\lambda = 3.7$, EGR = 50%.

Similar effect was observed for the point corresponding to $\lambda = 3.7$, EGR = 50% and is shown in Figure 27. This effect of cyclic variation on combustion has been observed in an experimental study elsewhere [18]. Comparing this behaviour with the in-cylinder temperature evolution (with respect to the number of cycles) at a point corresponding to $\lambda = 3.5$, EGR = 1%, a very low cycle-to-cycle variation was observed as expected (Figure 28).

The CO and HC emissions are sensitive to the cyclic variations in temperature. Hence, in accordance with the experimental procedures, an average over 10 cycles was used to evaluate the emissions for the points near the misfire boundary.

CONTROL OPTIONS

In this section two control options, namely trapping residual burned gas by variable valve timing and intake charge heating have been investigated. For this, the fuel flow rate (7.5 mg/cycle) and other model parameters discussed in Table 2 are kept constant.

Recently, these two control techniques have been compared for a direct injection HCCI engine [19]. There is, however, a substantial difference since port injection injects fuel into fresh air, while during direct injection, the fuel mixes with residuals trapped during negative valve overlap. As a consequence the study focused on the distribution of temperature, residual burned fraction and equivalence ratio for the aforementioned techniques, while no consideration was given to the combustion parameters and emissions.

VALVE TIMING: TRAPPING RESIDUAL BURNED FRACTION

External EGR works well due to its simplicity but its thermal effect is limited due to the heat loss in the EGR system and slow response during transient time. In comparison retaining the exhaust residual gas in the cylinder via cam phasing can avoid many of the system issues encountered with the external EGR approach [20]. Such trapping of residual gas in a four-stroke HCCI engine emulates the in-cylinder conditions of a two-stroke engine. The thermal energy of the trapped residual gas enhances auto-ignition [21]. Furthermore, this approach does not need high compression ratios or a heater to increase the charge temperature, thus enabling a switching over from SI to HCCI mode of operation. However, with the engine operated unthrottled and at very low loads there is not enough thermal energy within the exhaust gas to achieve auto-ignition [22].

The residual burned fraction is a technique exploited by many researchers to control auto-ignition timing. The induction of HCCI without intake air heating or very high compression ratios, by modifying the conventional valve timing of a port injected four-stroke SI engine (CR=10.3:1) to late IVO and early EVC, has been demonstrated [23]. HCCI mode was observed to produce low NO$_x$ and high unburned HC emissions at $\lambda = 1$, and fuel consumption during HCCI was comparable with that during SI operation. In a study involving two-stroke and four-stroke configurations and varying the residual gas rate was concluded as the main factor for convergence towards favourable 2-stroke conditions for auto-ignition [24]. Using mechanical valve actuation based on a camshaft with removable cams, the exhaust valve timing was observed to expand the operating range of auto-ignition towards higher load conditions. Two fundamentally different methods for controlled auto-ignition comprising of a more sophisticated active valve train that alleviate the necessity of intake charge heating and enable probing cam-less engines, have been introduced [25]. First, a sequential method employed
trapping of residual burned fraction by late closing of the exhaust valve and re-compressing the fresh intake charge with the residual burned fraction. In the second method, at the commencement of the induction stroke both inlet and exhaust valves were opened simultaneously thus drawing fresh charge as well as exhaust gases into the cylinder (re-breathing). With both the methods the pressure profiles obtained were similar and the amount of residual burned fraction determined the combustion initiation point. In case of the re-breathing method, significant heat loss at the exhaust port resulted in poorer preservation of the thermal energy compared to that in the re-compression method. In another study HCCI combustion was achieved with residual gas trapping (46-65 %) using variable cam timing [26].

The transition from SI to HCCI combustion on increasing the amount of residual gas fraction by increasing the negative valve overlap of the EVC with IVO symmetrically, has been demonstrated experimentally [27]. With equivalence ratios maintained in the range 1 and 0.77, HCCI mode offered clear benefit in terms of reduction in CO and NO\textsubscript{x} emissions and fuel consumption, compared to the SI operation. In another study, a four-stroke, naturally aspirated, camless HCCI engine with early EVC was used while predicting cyclic variations [18]. Sensitivities of exhaust and intake valve timings on the mass exhaled and inhaled have been investigated [28]. They implemented a single zone based full cycle model to simulate a PRF fuelled HCCI combustion. The EVC timing was observed to strongly influence the mass flow rates at intake and exhaust and hence the load. Whereas, IVO timing affected pumping losses significantly. The low pumping loss achievable due to gas exchange was beneficial in terms of fuel economy improvement at part load. In the same work, moderate intake air heating was observed to reduce the requirement of the EGR and thus widen the operating range at light load. The effect of increased trapped residual with negative valve overlap on HCCI combustion has been systematically simulated [29]. A segregated sequential CFD-driven full cycle model was adopted to simulate natural gas fuelled HCCI combustion. With increase in the negative valve overlap, a large amount of residual burned fraction (up to 66 %) was trapped in the cylinder and less fresh charge was introduced. This hot fraction resulted in an increase in the temperature just before EVO. In addition, the trapped residual burned gas contained appreciable oxygen thus lowering the equivalence ratio. Due to these conditions, the onset of combustion was advanced, but the peak temperature was lower due to the low equivalence ratio (dilution effect). However, in order to save the computational expense, a computational grid inadequate to account for boundary layer and crevice was used. Furthermore, a need to account for the inhomogeneities in composition and temperature was emphasized and mixing has been argued to be a crucial parameter in modelling HCCI combustion especially with a high residual burned fraction. In an extension to this study, inhomogeneity in composition was implemented, in addition to the inhomogeneity in temperature [30]. An interesting result for a high residual burned fraction trapping (42 %), showed that for a high average in-cylinder temperature condition the effect of temperature inhomogeneity nullified that of composition inhomogeneity. However, in the marginal combustion case (ignition timing delayed and combustion duration extended), the pressure profile predicted was different than the equivalent prediction in their previous work. Recently, the effect of the intake temperature on HCCI operation with negative valve overlap in a four-stroke port injected engine has been investigated [31]. At high load condition, the change in the intake temperature was observed to have only a modest impact, as the temperature of the trapped residuals was much higher than the intake temperature.

<table>
<thead>
<tr>
<th>Table 3: Inlet and exhaust valve timings</th>
</tr>
</thead>
<tbody>
<tr>
<td>VT1</td>
</tr>
<tr>
<td>IVO (°)</td>
</tr>
<tr>
<td>IVC (°)</td>
</tr>
<tr>
<td>EVO (°)</td>
</tr>
<tr>
<td>EVC (°)</td>
</tr>
<tr>
<td>RBF (%)</td>
</tr>
</tbody>
</table>

In the present study, the PDF based full cycle model was applied to investigate the effect of trapped residual burned fraction using late IVO and early EVC. The EGR valve was completely closed to study the effect of residual burned fraction (RBF) alone. The inlet and exhaust valve timings are given in Table 3.

![Figure 29: Valve timings.](image-url)
The valve timing events are depicted in the Figure 29. Increasing the negative valve overlap led to larger amount of trapped residual burned fractions in the engine cylinder. In this study, the fuel flow was maintained constant at 7.5 mg/cycle. Thus with increasing residual burned fractions, the amount of air is reduced i.e., the air-fuel ratio, $\lambda$ decreases as the overlap is increased. Hence the dilution effect of EGR is overshadowed by the constant fuel flow rate and the increased temperature of the residuals.

Figure 30: Effect of variable valve timing on the in-cylinder temperature.

Figure 30 depicts the in-cylinder temperature variation for various valve timing events. The hot trapped residual fraction advanced the auto-ignition of the air-fuel charge leading to higher peak temperatures. The smallest second hump observed in the temperature profile following the gas exchange process is present even during positive overlap and with 19% residual burnt fraction. With an increasing negative valve overlap, the amount of residual burnt fraction trapped surges. Thus the temperature at the second hump caused by the re-compression of the trapped residual burned gas fraction increases rapidly.

The pressure during compression (Figure 31) was the same for all the four valve timing events in agreement with that reported in ref. [29]. The CO and HC emissions reduced with increase in the in-cylinder temperatures, whereas the temperature sensitive NOx emissions increased as shown in Figure 32.

INTAKE CHARGE HEATING

The inlet charge temperature, i.e., the charge conditions at IVC is a convenient and efficient way to control the auto-ignition timing. This approach combined with variable compression ratio has been widely used for earlier four-stroke HCCI development on account of its effectiveness and practicality in controlling auto-ignition timing [1,32,33]. This method is the most widely applied HCCI control approach as the auto-ignition timing is very sensitive to intake charge temperature [34,35,36]. The high intake temperature triggers the onset of low-temperature (cool flame) chemistry, in turn reducing the main stage ignition delay. In addition at low loads, with the intake temperature strongly influencing the CO emissions, have emphasized the need of intake charge
heating to control the CO and HC emissions has also been emphasized [37].

However, this technique also has some drawbacks: For multi-cylinder engines, this control-option requires a very large power supply. Second, the thermal inertia of the cylinder wall and the intake manifold makes it difficult to change the inlet air temperature from cycle to cycle. Furthermore in case of vehicle applications, unless the exhaust gas energy is utilized to provide the required heat, this method is considered as impractical [28].

Figure 33: The effect of intake charge heating on the in-cylinder temperature.

In this section, the original valve timing (VT1) given in Table 1 was used, and the temperature at IVC was raised in steps of approximately 11 K. An increase in the intake temperature advanced the auto-ignition, increased the peak temperatures (Figure 33) and reduced the CO and HC emissions (Figure 34).

With the negative valve overlap, the thermal energy from the re-compression of the trapped residual gas, is available for advancing the auto-ignition timing during power stroke, in-turn raising the combustion temperature. These effects raise the temperature at the exhaust (Figure 29). This effect is absent in the case of intake charge heating. The potential problem of low exhaust temperatures of an HCCI engine while using oxidation catalysts for CO and HC emissions reduction was emphasized in ref. [38]. The high exhaust temperatures obtained with negative valve overlap have the potential to enable the use of a conventional oxidation catalyst for reducing the CO and HC emissions, in agreement with the results demonstrated experimentally elsewhere [23,31,37].

However, at very light loads, the temperature rise due to trapped residual gas is not high enough to trigger auto-ignition. In such situations, a combination of the two techniques i.e., using intake heating with negative valve overlap could be helpful.

![Figure 34: The effect of intake charge heating on the CO, HC and NOx emissions.](image)

With both the techniques, the increase in the in-cylinder temperatures reduced the HC and CO emissions and increased the NOx emissions, in agreement with the experimental observations [33,39].

**CONCLUSION**

HCCI operation in a PRF-fuelled, single cylinder, four-stroke HCCI engine with exhaust gas recirculation was modelled using the PDF based engine cycle model. The model predictions for the in-cylinder temperature and HC emissions were validated against the measurements for a base case, and showed a satisfactory agreement.

Furthermore, the model was implemented to develop an operating window for various combustion and emission parameters as a function of the amount of EGR and the air/fuel ratio. The model predictions for all the parameters investigated over the entire operating range, were compared with the experimental results. This rigorous validation test, and a reasonably good agreement between the trends as well as the magnitudes of predicted and experimental quantities, suggested the robustness of the model for simulating the HCCI operation. The three boundaries of a stable HCCI operation, namely the partial burn, knock, and misfire were reliably predicted by the model. The occurrence of knock was described in terms of the excessively rapid rate of pressure rise. The partial burn boundary was denoted by a very low IMEP and high CO and HC emissions. The model provides an insight into misfire phenomenon and a possible way it could be accounted...
for while modelling HCCI operation. The misfire was demonstrated by considering a multiple cycle simulation where the intake charge failed to burn during some of the cycles.

Thus, the integrated PDF based model serves as an efficient tool to construct and understand the operating window for HCCI engines. Such operating windows can be developed for various fuels and compared, while studying the influence of the type of fuel on HCCI characteristics. With the inclusion of detailed chemistry, the PDF based model is applicable over the entire range of operating conditions, in comparison to the reduced mechanisms which are valid only for a limited range of thermodynamic conditions. Additionally, an operating window is useful for estimating the effect of various control parameters on the expansion of the operating window to high loads.

Finally, two control options, i.e., residual burned fraction trapping by variable valve timing and intake charge heating were investigated. The usefulness of negative valve overlap in obtaining higher exhaust gas temperatures, thereby enabling the use of conventional CO and HC removal oxidation catalysts was demonstrated. However, the need for a combination of the two control techniques at light loads was pointed out. As a result, theoretically, a possible control strategy for HCCI engine can be identified as: at very low loads intake temperature heating with some residual gas trapping; at low to medium loads residual gas trapping alone; and at high loads SI operation, could enable a stable engine operation over the entire operating range. Such a hybrid operation with SI is possible as the intake temperature and residual burned gas ensure that the in-cylinder conditions are right for auto-ignition without any need for increasing the compression ratio, thus facilitating the hybridization with a low compression ratio SI mode.

ACKNOWLEDGMENTS

The authors would like to thank Kayiu Man at Brunel University, and Steven Liput at the University of Cambridge for their help in representing the experimental set up on the 1-D code interface. The authors are grateful to the Centre for Scientific Enterprise Ltd. for their financial support.

REFERENCES

1. Thring, R. H., Homogeneous Charge Compression Ignition (HCCI) Engines”, SAE 892068.


CONTACT

Dr Amit Bhave
Presently at:
Reaction Engineering Solutions Ltd., UK.
amitbhave@resolutionsltd.com

Dr Markus Kraft
University of Cambridge, UK.
mk306@cam.ac.uk

Prof Fabian Mauss
Lund Institute of Technology, Sweden.
fabian.mauss@forbrf.lth.se

Prof. Hua Zhao
Brunel University, UK.
hua.zhao@brunel.ac.uk

NOMENCLATURE

ABDC  After bottom dead center
AFR  Air-fuel ratio
ATDC  After top Dead Center
BBDC  Before bottom dead centre
BTDC  Before top dead center
CAD  Crank angle degrees
Stochastic fluctuation parameter

Compression ratio

diameter of a pipe in the set-up

Exhaust gas recirculation

Exhaust valve closure

Exhaust valve opening

Homogeneous charge compression ignition

Indicated mean effective pressure

Inlet valve closure

Inlet valve opening

Length of a pipe in the set-up

Number of stochastic particles

Probability density function

Particulate matter

Primary reference fuel

radius at a bend.

Revolutions per minute

Spark ignition

Stochastic reactor model

In-cylinder temperature

In-cylinder temperature at IVC

Wall temperature

Actual air–fuel ratio / stoichiometric air-fuel ratio

Characteristic mixing time parameter