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A Detailed Chemistry Simulation of the SI-HCCI Transition

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Abstract

A Stochastic Reactor Model (SRM) has been used to simulate the transition from Spark Ignition (SI) mode to Homogeneous Charge Compression Ignition (HCCI) mode in a four cylinder in-line four-stroke naturally aspirated direct injection SI engine with cam profile switching. The SRM is coupled with GT-Power, a one-dimensional engine simulation tool used for modelling engine breathing during the open valve portion of the engine cycle, enabling multi-cycle simulations. The model is initially calibrated in both modes using steady state data from SI and HCCI operation. The mode change is achieved by switching the cam profiles and phasing, resulting in a Negative Valve Overlap (NVO), opening the throttle, advancing the spark timing and reducing the fuel mass as well as utilising a pilot injection. Experimental data is presented along with the simulation results. The model is used to investigate key control parameters and their effects on parameters that are difficult to measure experimentally. The effect of the spark in the first HCCI cycles is found to have a major impact on the stability of the transition.

Contents

1 Introduction

Homogeneous Charge Compression Ignition (HCCI) is an Internal Combustion Engine (ICE) operating mode with the potential to reduce emissions and improve efficiency compared with conventional engine operating modes. It is characterised by low temperature fuel oxidation that occurs throughout the engine cylinder in a short period of time. HCCI engine operation can be achieved by many different strategies and by using a large variety of fuels. Here we focus on HCCI in a spark ignition engine that utilises a Negative Valve Overlap (NVO) to achieve auto-ignition of a gasoline fuel as this is perhaps the most practical method for realising commercially viable HCCI engines.

HCCI does however suffer from a limited operating range. The low load limit occurs during start up and when the fuel concentration is too low to ignite properly leading to unstable operation. Due to the rapid rate at which the chemical energy of the fuel is released in HCCI operation there is also a high load limit. To overcome this problem it is possible for the engine to switch from HCCI to SI mode when the high or low load limit of HCCI is reached. This can be achieved by rapid switching of the cam profiles [1]. Shorter valve opening durations and lower lifts are used in HCCI mode, resulting in an NVO that traps hot residual gas in the cylinder. Consequently the IVC temperature is high enough for HCCI to occur. An exhaust gas re-breathing strategy may also be used with similar effects [2].

Switching between HCCI and SI operation is non-trivial due to the different in-cylinder conditions in each mode. The Exhaust Gas Recycle (EGR) ratio in HCCI mode is usually around 40-60 % [3]. The temperatures in the two modes are also very different. Several researchers have looked at ways of achieving the transition smoothly however there is still considerable work to be done before HCCI will be commercially viable. Some researchers have found switching from SI mode to HCCI mode more difficult due to the high temperatures in SI mode [1, 3]. Others have found the opposite to be true due to the slow drop in inlet pressure when the throttle is closed [4]. The region between SI and HCCI combustion with intermediate EGR ratios was found to be unstable and suffers from cycle to cycle variations [5–7]. Operating with spark ignition during stable HCCI was found to make little difference but during the transition it can greatly stabilise the combustion [8, 9].

Engine modelling can be used as a useful tool to gain insight into the complex processes that occur in an engine. Parameters that are difficult to measure and their effects can be investigated using simulations and the results can provide helpful directions for experimental work as well as optimising control [10]. Computational Fluid Dynamics (CFD) is a useful modelling tool for providing detailed insight into in-cylinder turbulence and mixing. CFD however is computationally expensive and generally limited to single-cycle single-cylinder investigations. The importance of the chemical kinetics in auto-ignition combustion makes it highly beneficial to use a detailed chemical mechanism when modelling HCCI. Probability Density Function (PDF) based models have proved an advantageous tool in modelling HCCI combustion due to the incorporation of detailed chemistry whilst maintaining relatively low computational times [11].

The transition between SI and HCCI is even more challenging to model, and the different

operating modes produce unusual temperatures, pressures and compositions at IVC in each cycle and cylinder during the transition. A mixture between SI and HCCI combustion has been reported during the transition and simulated using a double Wiebe function [**?**]. In this paper we present SI-HCCI simulation results from a detailed chemical kinetic model, previously used to simulate both SI and HCCI engine operation [11–15].

The aim of this paper is to describe the computationally efficient detailed chemistry model used to simulate the transition from SI to HCCI and to investigate the results. We first present details of the engine and the method by which the transition is achieved. The following section introduces the model and describes how it has been set-up to simulate the transition. Next we present the calibration of the model in both HCCI and SI operation. The results from the multi-cylinder simulation of the transition are presented and finally we draw conclusions.

2 Experimental Details

The transition from SI-HCCI was made at 2.2 bar BMEP and 1500 rpm in a 4-cylinder, in-line, naturally aspirated Gasoline Direct Injection (GDI) SI engine equipped with two-stage profile camshafts. Details of the engine are given in Table 1 and more information about the experiments can be found in [16].

Table 1: *Engine specifications.*

Cylinders	4
Fuel	95 RON gasoline
Bore [mm]	87.5
Stroke [mm]	83.0
Con. Rod Length [mm]	146.3
Disp. volume [cm^3/cyl]	499
Compression Ratio	12

Figure 1 shows the in-cylinder pressure, inlet manifold pressure and valve lifts during a transition from SI to HCCI. The transition is achieved by switching the cam profiles resulting in shorter valve opening durations and lower lifts. The cam phasing is also advanced to increase the amount of hot residual exhaust gas trapped in the cylinder. In HCCI mode the throttle is opened resulting in a lean cylinder charge. The cam profile switch takes place in the cylinder firing order 3-4-2-1.

Table 2 gives details of steady state SI and HCCI operating conditions. Less fuel is required in HCCI due to the higher efficiency achieved compared with SI mode. In steady HCCI mode a split injection strategy was used, in which 20 % of the fuel was injected during NVO, referred to as pilot injection. The pilot injection timing was 45 CAD before intake TDC. The second, main injection, took place during the intake stroke.

The crank angle notation adopted here is to use combustion TDC as 0 CAD and NVO TDC as 360 CAD. The cycle is assumed to start at IVO (a negative number) and end at

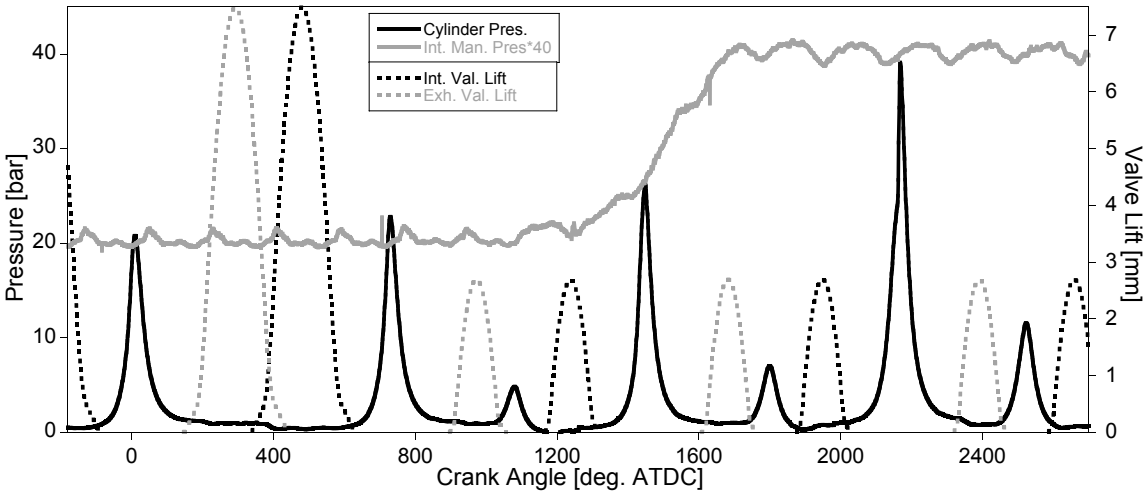


Figure 1: *In-cylinder pressure, inlet manifold pressure and valve lifts during a transition from SI to HCCI.*

Table 2: *Steady state operating conditions.*

Mode	SI	HCCI
Equivalence Ratio	1.0	0.71
Fuel Mass [mg/cyl/cyc]	8.81	8.51
Fuel Split Ratio	1.0	0.8
Main Injection [CAD ATDC]	-310	-260
Pilot Injection [CAD ATDC]	-	315
EGR Ratio [%]	30.1	51.5
Spark Timing [CAD ATDC]	-46	-32
Throttle Opening [Deg.]	4.6	50.0

the following IVO (a positive number). When a cycle's NVO is referred to, it is therefore the NVO following the combustion of that cycle.

During the transition the injection timings, spark timings and fuel mass are varied. In the final SI cycle, the spark is advanced to -55 CAD ATDC and the fuel amount increased to 11.3 mg/cyl/cyc. The first two HCCI cycles are also controlled differently compared with steady state HCCI. The spark timing is advanced to -60 CAD ATDC and the pilot injection timing is retarded to 360 CAD ATDC. The fuel mass is reduced to 8.3 mg/cyl/cyc, however the fuel split ratio was maintained at 80 %. The parameters were chosen by manual optimisation to produce a smooth transition. Although a spark was used in stable HCCI it was found to have no influence on the combustion at the highly diluted conditions investigated.

A fast Universal Exhaust Gas Oxygen (UEGO) sensor, with a response time of 10-20 ms, was used to measure the air fuel ratio in the exhaust port of cylinder 4. In cylinder CO_2 volume fraction was measured using two Non-Dispersive Infrared (NDIR) sensors. This

enabled calculation of the EGR ratio by assuming that all of the CO_2 present in the compression stroke was produced in the previous combustion. Full details of these experiments are given in [16].

3 Model Details

The Stochastic Reactor Model (SRM) is a spatially zero dimensional model based on Probability Density Function (PDF) transport methods [17]. The cylinder charge is split into an ensemble of notional particles that make up the PDF of temperature, pressure and composition space. In-cylinder turbulent mixing is accounted for using the Euclidean Minimum Spanning Tree (EMST) sub-model [18]. Stochastic heat transfer and direct injection sub-models are also included. An important feature of the model is the detailed Primary Reference Fuel (PRF) chemical mechanism containing 157 species and 1552 reactions [11, 14, 15].

The SRM was coupled with GT-Power, a one dimensional engine simulation tool, to enable multi-cycle simulation. GT-Power was used to model heat and mass flow through the engine during the intake and exhaust events and user models were added to control the throttle and valve lifts. The SRM is used to simulate in-cylinder mixing, heat transfer and chemistry during the closed valve events.

The engine was previously modelled in HCCI mode at a slightly higher load and changes in injection timing as well as fuel split were studied in detail [13]. Here we present some of the key assumptions. The main fuel injection takes place during the intake stroke and is assumed to result in a homogenous mixture at IVC. For this reason all particles at IVC were specified with the same composition, temperature and pressure. The cooling effect of spray evaporation was however not ignored and was accounted for at IVC. Due to fluctuations in air and EGR mass in each cycle, the fuel mass rather than the equivalence ratio was set and the EGR mass instead of ratio was used. This meant that equivalence ratio and EGR ratio were predictions that could be used to validate the model. The composition and mass at IVO was stored and used as EGR for the following IVC event. The composition of EGR at EVO was also stored and used as the initial composition at EVC.

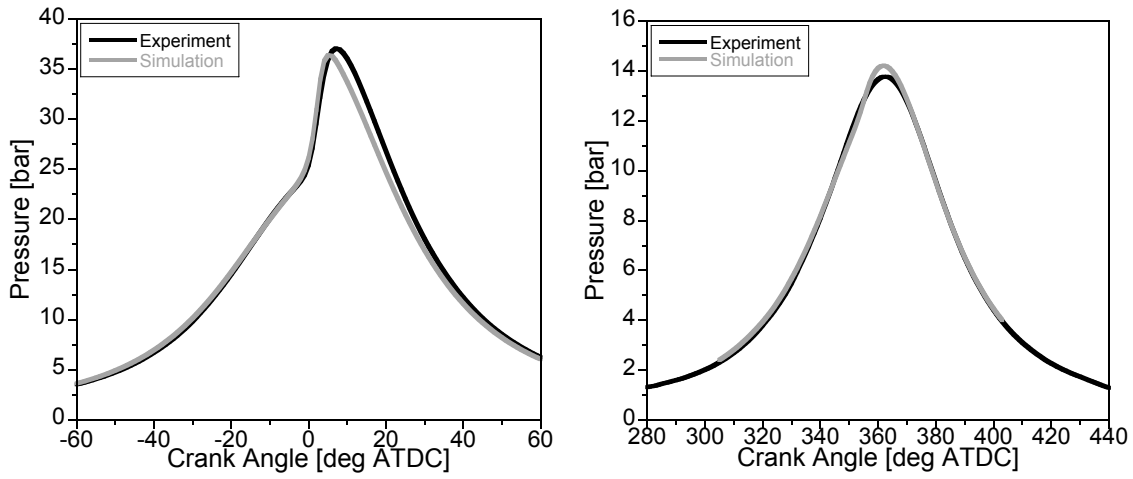
The SRM has also been developed to enable SI simulation. It is assumed that the flame is a sphere and centred at the spark location. In SI mode the particle ensemble is split into three zones; unburned, entrained and burned. Mixing occurs within each zone but not between them. The entrained volume is calculated using a turbulent flame speed correlation and particles are moved from the unburned zone into the entrained zone accordingly. The freshly entrained particles mix with burning entrained particles and begin to combust. When a particle's heat release rate has dropped below a set value it is transferred to the burned zone. The value, $1109\,\mathrm{J.kg^{-1}.s^{-1}}$, was determined through calibration of the model. The detailed chemical mechanism is used in every particle in each of the three zones. This has resulted in very good NO_x prediction and enables simulating the auto-ignition of the end gas. This was found to be necessary when modelling the SI-HCCI transition as a mixture of the two combustions can occur in the early transient cycles. In SI mode the EGR mass was assumed constant, however the EGR composition was updated every cycle. As the unburned gas may auto-ignite before being consumed by the

flame, if the unburned gas temperature rises above 1500 K the flame propagation model is switched off and all particles returned to a single zone. This enables simulation of spark assisted HCCI. Full details of the model can be found in [12].

4 Model Calibration

The model was calibrated in HCCI and SI operating modes on the same GT-Power engine map. This was a difficult task and required extensive calibration to make sure the IVC pressures and temperatures were adequate when the valve and throttle changes were made.

Experimental measurements reported 30 % EGR in SI mode, when there is no NVO. This is caused by the low inlet manifold pressure and the exhaust and inlet valves being open at the same time. From the EGR ratio, fuel mass, equivalence ratio, volume and measured pressure, an estimate for the IVC temperature can be made. The model was calibrated by varying valve discharge coefficients and wall temperatures within reasonable limits to obtain the required temperatures and pressures at IVC and EVC. In SI mode the entrainment rate constant used in the empirical correlation for flame speed was varied to obtain the correct heat release rate. More details of this can be found in [12]. The heat release rates were also affected by mixing times that were varied within sensible bounds. At IVC the composition and temperature of the cylinder charge was assumed to be homogeneous in both SI and HCCI due to the early injection of fuel during the intake stroke. EGR compositions are taken from the in-cylinder composition at the previous valve opening event.



(a) Main Combustion. (b) NVO.

Figure 2: *Comparison of averaged experimental and simulated HCCI pressure profiles.*

4.1 HCCI Calibration

The model was calibrated in HCCI mode at the speed and load of the transition. The pressure profiles, in Figure 2 below, show profiles averaged over 96 experimental and 50 simulated cycles and a good agreement between the experiment and simulation. The EGR ratio was 47.0 % and 51.7 % in the simulation and experiment respectively. The equivalence ratio was 0.67 and 0.71 in the simulation and experiment respectively. This is a good indication that the temperatures and pressures at EVC and IVC are similar in the experiment and simulation.

4.2 SI Calibration

The model was calibrated at the speed and load of the transition in SI mode. Figure 3 compares an SI cycle with an average peak pressure with a steady state simulated SI cycle. The simulated pressure profile matches the experimental profile well.

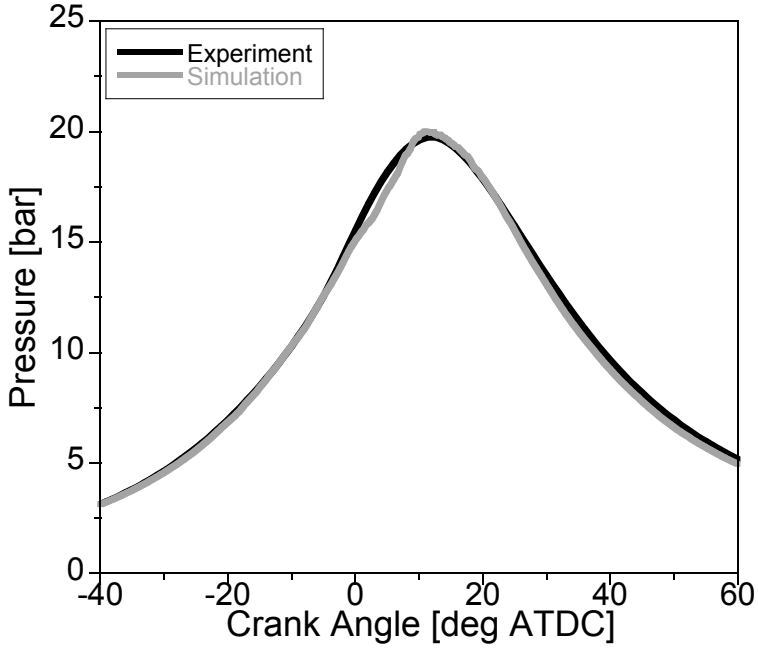
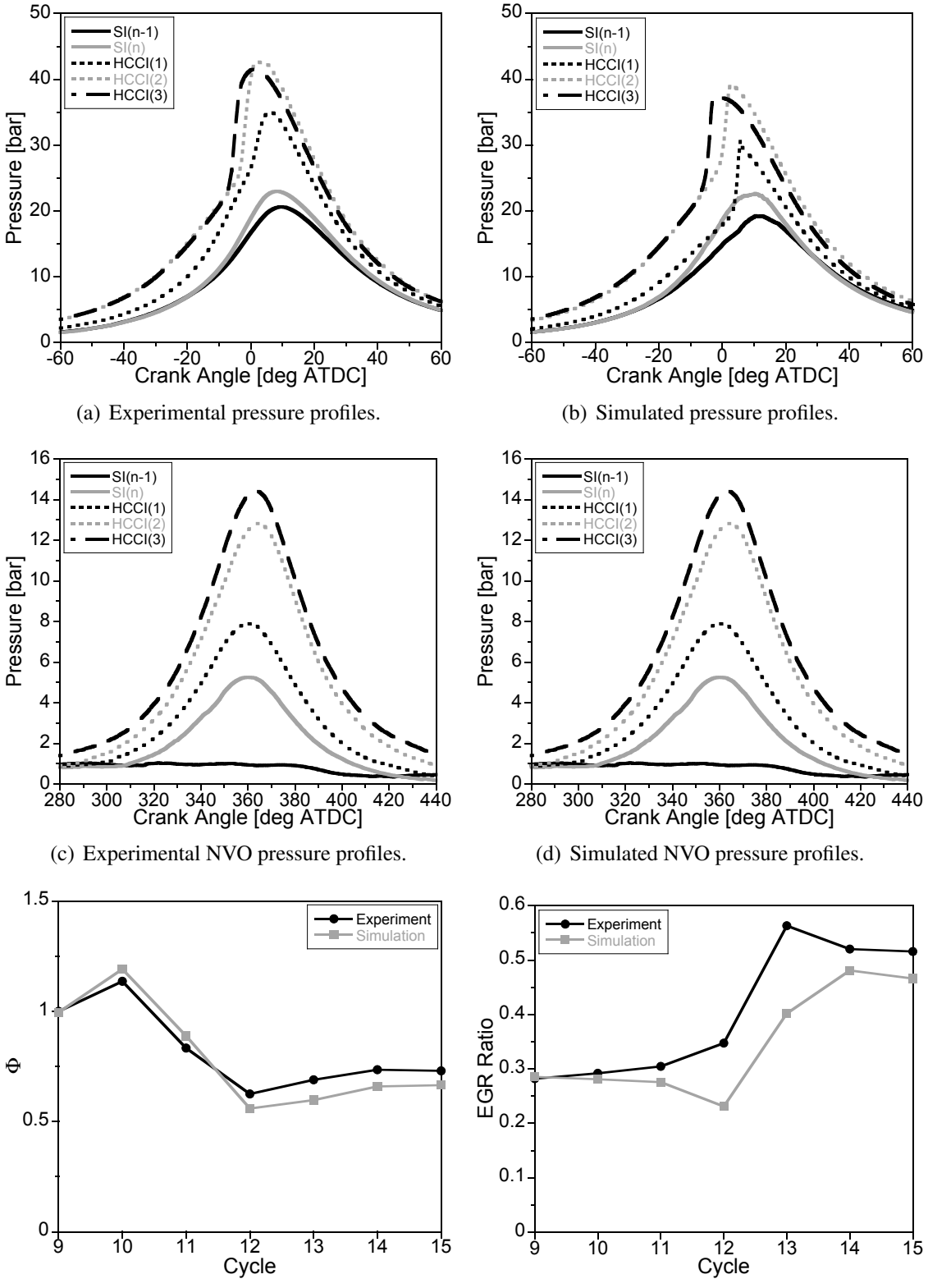


Figure 3: *Comparison of SI pressure profiles from experiment and simulation.*

5 Results

5.1 SI-HCCI Transition

EGR ratio and equivalence ratio were measured on a cycle to cycle basis in cylinder 4. For this reason we present a comparison of experimental and simulated results from



(a) Experimental pressure profiles.

(b) Simulated pressure profiles.

(c) Experimental NVO pressure profiles.

(d) Simulated NVO pressure profiles.

(e) Equivalence ratio during transition.

(f) EGR ratio during transition.

Figure 4: *Comparison of experimental and simulation results from cylinder 4. The final SI cycle is number 10.*

cylinder 4 in this section. Figure 4 compares results obtained in the detailed simulation with experimental results in cylinder 4. Figures 4a and 4b show the in-cylinder pressure obtained from the experiment and simulation respectively. The pressure profiles match the experimental data extremely well for a transient engine simulation. The final SI cycle, SI(n), exhibits a faster pressure rise and a higher peak pressure than the previous cycle due to the addition of extra fuel and an earlier spark timing in this cycle compared with steady state SI. The following cycle, HCCI(1), is a mixture of flame propagation and auto-ignition. Without the spark the cycle was found to misfire. The inlet valve closes earlier due to the cam profile switch causing an increase in the compression pressure. Flame propagation occurs until around TDC when the remaining unburned fuel auto-ignites. The decrease in fuel air equivalence ratio in the 2^{nd} and 3^{rd} HCCI cycles hinders flame propagation, causing more HCCI like combustion to occur, although flame propagation is still important in the 2^{nd} cycle due to a low IVC temperature.

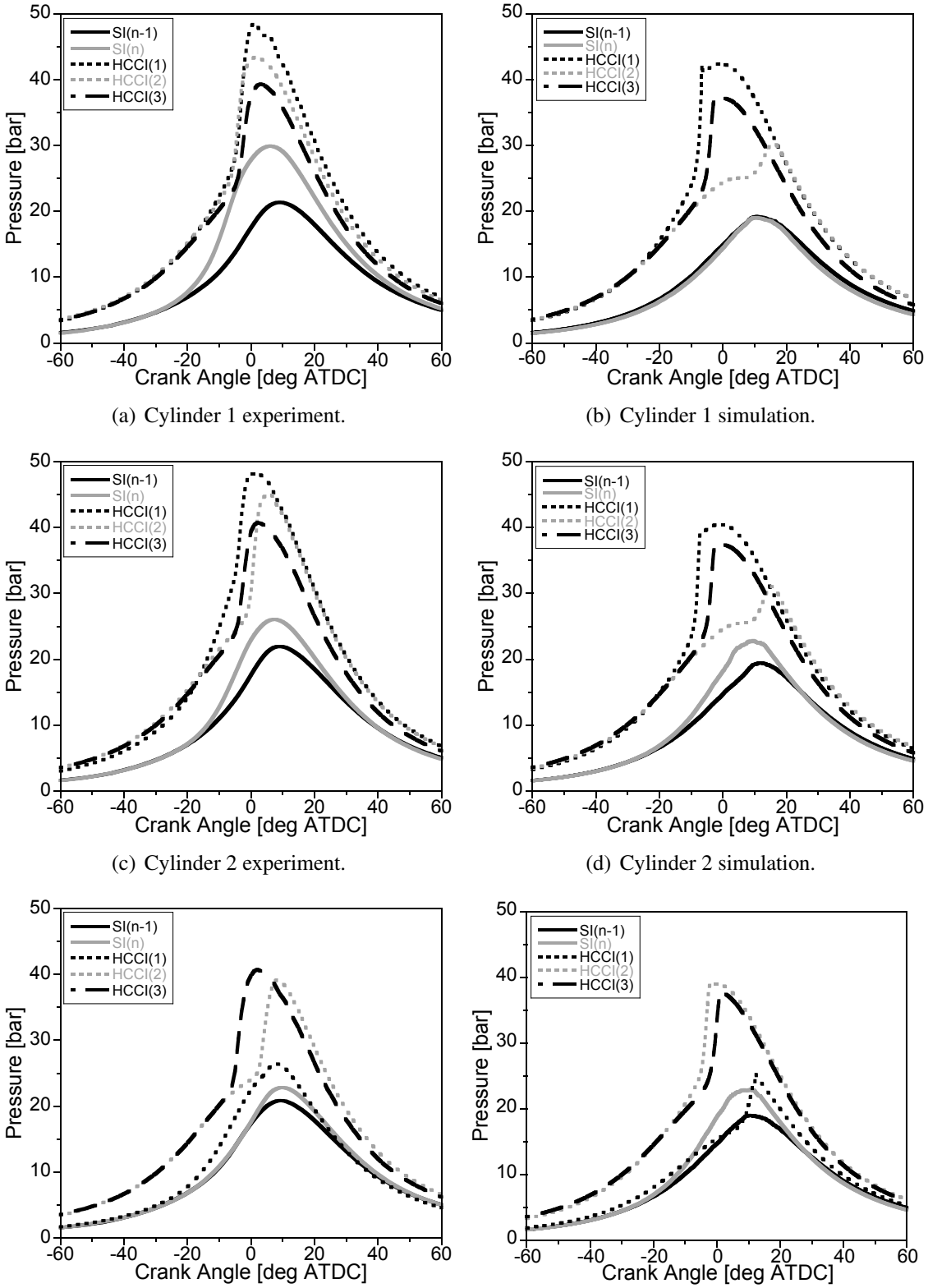
Figures 4c and 4d show the experimental and simulated NVO pressure profiles during the transition respectively. The NVO peak pressure increases in consecutive cycles due to the advance in the EVC timing. Little NVO heat release occurs in the first two NVOs due to the low amount of O_2 present.

The equivalence ratio in cylinder 4 during the transition is shown in Figure 4e. In cycle 10, the last SI cycle, the cylinder charge becomes rich as an increased amount of fuel was injected compared to steady state SI. The value then drops in the following two cycles as the injected fuel mass is decreased and the throttle is opened and the inlet valve closes earlier trapping more air in the cylinder. The mass of fuel is then increased, which is shown by the increase in equivalence ratio in both the experiment and simulation.

Figure 4f shows the measured and simulated EGR ratios in cylinder 4. The CO_2 volume fraction during exhaust and compression stroke was measured and used to calculate the EGR ratio. It is assumed that all of the CO_2 present during compression originated from the previous combustion. This does not however take into account the small amount of CO_2 produced during NVO. This would suggest the measurement is slightly higher than the actual value after cycle 10. The simulated EGR ratio is slightly lower than the measured value and this may be due to the above reason. Although EVC is advanced, trapping increasing amounts of EGR, the EGR ratio initially drops. This is due to the throttle opening and IVC advancing, increasing the overall mass of cylinder charge. The IVC temperature also drops and contributes to this as will be described later. The EGR ratio then begins to increase as EVC is advanced and the exhaust temperature decreases.

5.2 Cylinder-to-Cylinder Variations

The combustion pressure profiles for the remaining cylinders are given in Figure 5. The transient behavior in all cylinders diminished within 5 cycles of the transition in both the experiment and simulation. Figure 6 gives more detail of the simulated transition in each cylinder. As mentioned above, due to the firing order (3-4-2-1), each cylinder undergoes different conditions during the transition as IVC is advanced and the throttle opened as well as the advance in EVC that traps an increasing amount of EGR until steady state is reached.



(a) Cylinder 1 experiment.

(b) Cylinder 1 simulation.

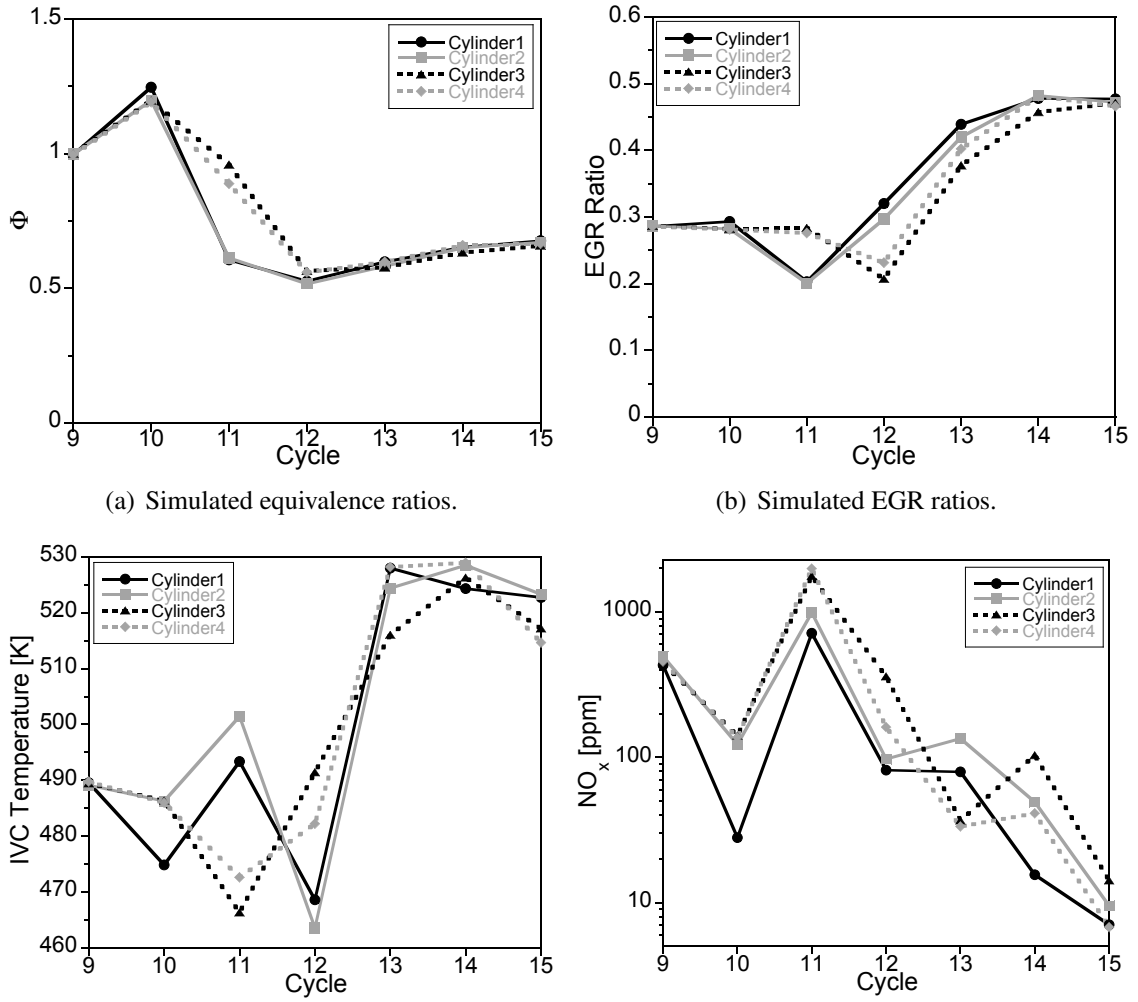
(c) Cylinder 2 experiment.

(d) Cylinder 2 simulation.

(e) Cylinder 3 experiment.

(f) Cylinder 3 simulation.

Figure 5: *Comparison of experimental and simulated pressure profiles.*



(a) Simulated equivalence ratios.

(b) Simulated EGR ratios.

(c) Simulated IVC temperatures.

(d) Simulated NOx emissions.

Figure 6: *Comparison of simulation results in each cylinder. The final SI cycle is number 10.*

The equivalence ratios in all 4 cylinders increase in the final SI cycle due to the increased mass of fuel injected (see Figure 6a). The first HCCI cycle, cycle 11, is the only cycle that shows a large difference in equivalence ratio for each cylinder. This is due to the throttle opening, causing the inlet manifold pressure to increase as well as the advance in EVC that traps increased amounts of EGR. In this cycle higher equivalence ratios are seen in cylinders that undergo the transition earlier. In the second HCCI cycle, cycle 12, the equivalence ratios all move towards a similar value that is leaner than in steady state HCCI. The cylinders that were richer in the previous cycle have lower EGR mass in cycle 12, due to the cam phasing, and this causes the equivalence ratio of all the cylinders to converge. This occurs even though the EGR trapped from the richer cycles will consequently be richer.

Figure 6b shows the EGR ratio in each cylinder during the transition. Due to the throttle opening, cylinders 1 and 2 have lower EGR ratios in the first HCCI cycle as the amount

of fresh charge is increased with inlet manifold pressure. EGR ratios then increase in the following cycles as the EVC timing is advanced, trapping larger amounts of EGR. The speed with which the cylinders' EGR ratio moves towards steady state is linked to the firing order with the later firing cylinders reaching steady state faster as the fluctuations in the intake decrease.

Figure 6c shows the IVC temperatures and similar trends following the firing order, 3-4-2-1, can be seen. The last SI cycle in cylinder 1 is affected by the throttle opening and has a lower IVC temperature which results in lower NO_x emissions, as shown in Figure 6d. NO_x emissions are highest in the first HCCI cycles due to the mixed SI-HCCI combustion and the large amount of fuel present. Although IVC temperatures in cylinders 3 and 4 are lower in this cycle compared with their previous SI cycles, the IVC is much earlier, resulting in higher peak temperatures and elevated NO_x emissions. NO_x emissions in subsequent cycles decrease as flame propagation becomes unstable and the re-circulated NO_x diminishes.

6 Conclusions

A stochastic reactor model (SRM) was used to simulate an engine in both HCCI and SI modes. The model was coupled with GT-Power to enable multi-cycle, multi-cylinder simulations with detailed chemistry. The transition from SI to HCCI was simulated and the results compared with experimental data. The simulated pressure profiles matched the trends in the measured values extremely well as well as the EGR ratio and equivalence ratio in cylinder 4.

The first HCCI cycle was found to be a combination of flame propagation and auto-ignition. Without the spark the simulation resulted in a misfire. The ability of the model to simulate auto-ignition at the same time as flame propagation with a detailed chemical mechanism resulted in a good fit to the experimental data.

The early intake valve closing in the 1^{st} HCCI cycle compared to steady state SI caused an increase in the temperatures reached, resulting in high NO_x emissions. Trends in the in-cylinder simulation results were found to follow the cylinder firing order.

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