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A Fast Detailed-Chemistry Modelling Approach for Simulating the SI-HCCI Transition

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Abstract

An established Stochastic Reactor Model (SRM) is used to simulate the transition from Spark Ignition (SI) to Homogeneous Charge Compression Ignition (HCCI) combustion 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 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 using a pilot injection. A proven technique for tabulating the model is used to create look-up tables in both SI and HCCI modes. In HCCI mode several tables are required, including tables for the first NVO, transient valve timing NVO, transient valve timing HCCI and steady valve timing HCCI and NVO. This results in the ability to simulate the transition with detailed chemistry in very short computation times. The tables are then used to optimise the transition with the goal of reducing NO_x emissions and fluctuations in IMEP.

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1 Introduction

Homogeneous Charge Compression Ignition (HCCI) is an internal combustion engine operating mode with the potential to improve efficiency and reduce emissions compared with standard operating modes. It is characterised by low temperature fuel oxidation that occurs throughout the engine cylinder in a short time. Many different strategies and a large variety of fuels have been used to achieve HCCI engine operation. The focus of this paper is HCCI in a spark ignition engine using a Negative Valve Overlap (NVO) to achieve auto-ignition of a gasoline fuel.

The limited operating range of HCCI is one of its main drawbacks. The low load limit occurs during start up and when the fuel concentration is too low to ignite properly causing unstable operation. The rapid rate of heat release in HCCI operation, which can lead to engine damage, is responsible for the high load limit. To overcome this problem it is possible for the engine to switch from HCCI to SI mode before the high load limit of HCCI is reached. Rapid switching of the cam profiles can be used to achieve this [1]. Shorter opening durations and lower lifts compared to those used in SI mode result in an NVO that traps hot residual gas in the cylinder, raising the IVC temperature so that HCCI engine operation can occur. An exhaust gas re-breathing strategy may also be used with similar effects [2].

The switch between HCCI and SI operation is complicated due to the different in-cylinder conditions in each mode. The Exhaust Gas Recycle (EGR) ratio in HCCI mode is typically between 40-60% [3]. The inlet valve closing (IVC) and exhaust gas temperatures in the two modes are also very different. A lot of research has gone into achieving a smooth transition however there is still a substantial amount of work to be done before HCCI becomes commercially viable. Some researchers have found it more difficult to achieve a stable transition when switching from SI mode to HCCI mode due to the high temperatures in SI mode [1, 3]. Others have found the switch from HCCI to SI mode more complicated because of 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 can improve the stability during a SI-HCCI transitions but was found to make little difference during stable HCCI [8, 9].

Engine modelling can help to gain insight into the complex processes that occur in an engine. Parameters that are difficult to measure experimentally can be estimated using computational models and their effects can be investigated. Simulation results can provide helpful directions for experimental work as well as optimising control [10]. When modelling HCCI engines it is very useful to use a detailed chemical mechanism due to the importance of chemical kinetics in auto-ignition combustion. Maintaining relatively low computational times whilst incorporating detailed chemistry can be achieved by using Probability Density Function (PDF) based models, making them an advantageous tool in modelling HCCI combustion [11]. A PDF based model has been used to simulate both SI and HCCI combustion with detailed chemistry [12, 13]. Challenges still remain in predicting spray and in-cylinder fluid motion in shorter simulation times. Improvements to chemical mechanisms to make them more predictive when modelling the combustion of real fuels and to shorten computation times are still difficult issues to overcome.

The transition between SI and HCCI is even more taxing to model, and the different operating modes produce unusual temperatures, pressures and compositions at IVC in each cycle and cylinder during the transition. A combination of SI and HCCI combustion modes has been reported during the transition and simulated using a double Wiebe function which allowed fast simulation of the transition for control purposes [7]. Real time simulation of HCCI engines using a detailed chemistry model has been achieved by using a tabulation technique [14, 15]. This paper presents a similar method that allows fast simulation of the SI-HCCI transition using a tabulated model containing detailed chemistry. The same technique could be used for the reverse transition, however this paper focuses on the transition from SI to HCCI.

The aim of this paper is to describe the optimisation method used to reduce NO_x emissions and fluctuations in IMEP during the transition from SI to HCCI. Initially details of the engine and the method by which the transition is achieved are presented. The following section introduces the model and describes how it has been tabulated to achieve fast simulation of the transition. Next the calibration of the model in both HCCI and SI operation is presented. The results from a multi-cylinder simulation of the transition are presented. Subsequently the output from an optimisation of the transition using the model is demonstrated and finally conclusions are drawn.

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 switch occurs in a single cycle and is controlled by adjusting the pressure of the oil entering the cylinder head. The exhaust cam is switched just before the intake cam. The cam phasing is also advanced to increase the amount of hot residual exhaust gas trapped in the cylinder. In HCCI mode the

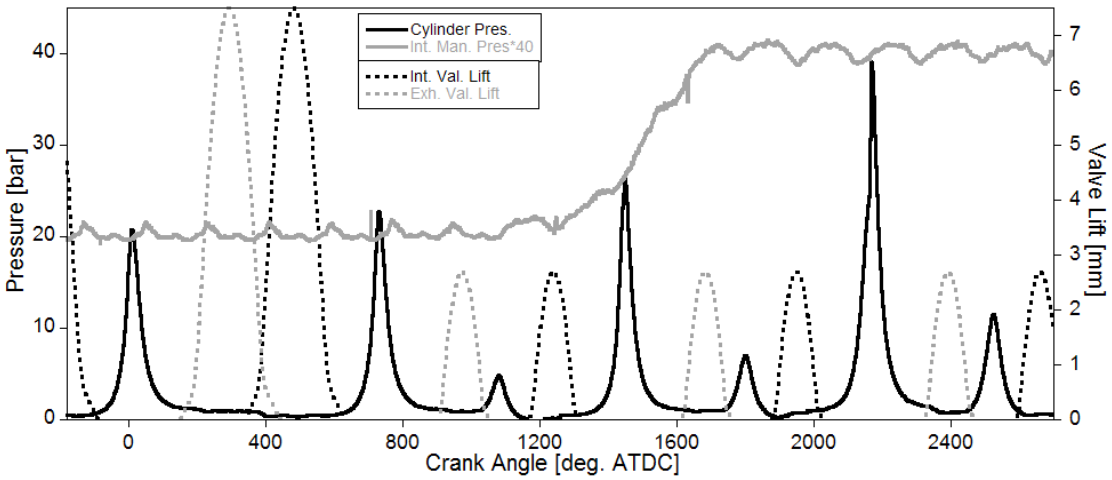


Figure 1: *In-cylinder pressure, inlet manifold pressure and valve lifts during a transition from SI to HCCI.*

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

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

A fast Universal Exhaust Gas Oxygen (UEGO) sensor was used to measure the air fuel ratio in the exhaust port of cylinder 4. In-cylinder CO2 volume fraction was measured us-

ing two Non-Dispersive Infrared (NDIR) sensors and the measurements used to estimate the EGR ratio. Details of these experiments are given in [16].

The mode switch is set up in 4 stages. Firstly there is steady state SI. The second stage is the final SI cycle, in which parameters may be set differently to those in steady SI. The next stage is two HCCI cycles that can be controlled differently to the final stage, the steady state HCCI. During the mode switch it is possible to control the fuel mass and spark timing as well as fuel split ratio and injection timings in each of the four stages. The timing the throttle is opened is also a useful control parameter.

3 Model Details

3.1 Stochastic Reactor Model

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 particles that make up the PDF of temperature, pressure and composition space. In-cylinder turbulence is accounted for using the Euclidean Minimum Spanning Tree (EMST) mixing model [18]. Stochastic heat transfer and direct injection sub-models are also included. A flame propagation model has also been added to enable SI simulation and full details are given in [12]. An important feature of the model is the detailed Primary Reference Fuel (PRF) chemical mechanism containing 157 species and 1552 reactions [12–14, 19, 20]. The full model has been used to successfully simulate the transition from SI to HCCI and results are presented in [21].

3.2 Tabulation

The SRM is relatively computationally cheap compared with other detailed chemistry modelling approaches, making it ideal for simulation on a multi-cycle, multi-cylinder basis. However, to run an optimisation of a process requires simulation of a large number of cycles and it would be impractical to use the SRM for this purpose. A previously developed tabulation scheme [14, 15], wherein a table is constructed by varying chosen input parameters to the SRM, is ideal for this use. A table can be created to store individual simulation results from the SRM and subsequently used to look up an interpolated SRM output when passed input parameters within the range of the table. The interpolation uses cubic natural splines to find the desired output from the table.

The SRM has been tabulated in order to increase the speed of simulation and enable optimisation of the mode switch. Due to the scaling of the number of simulations required to produce a table, the tabulation is limited to 4-5 input parameters. As the SRM has a much greater number of input parameters (157 species concentrations to start with), the input parameters have to be chosen carefully to reflect the transient behavior they must cover.

The switch from SI to HCCI operating modes is complicated to simulate, as two modes

of combustion are present along with the heat released during NVO. This means that different tables are required at different points in the transition so that suitable input parameters can be chosen at each stage of the mode switch, reducing the overall number of simulations required to build them, compared with an enormous table to encompass the in-cylinder events.

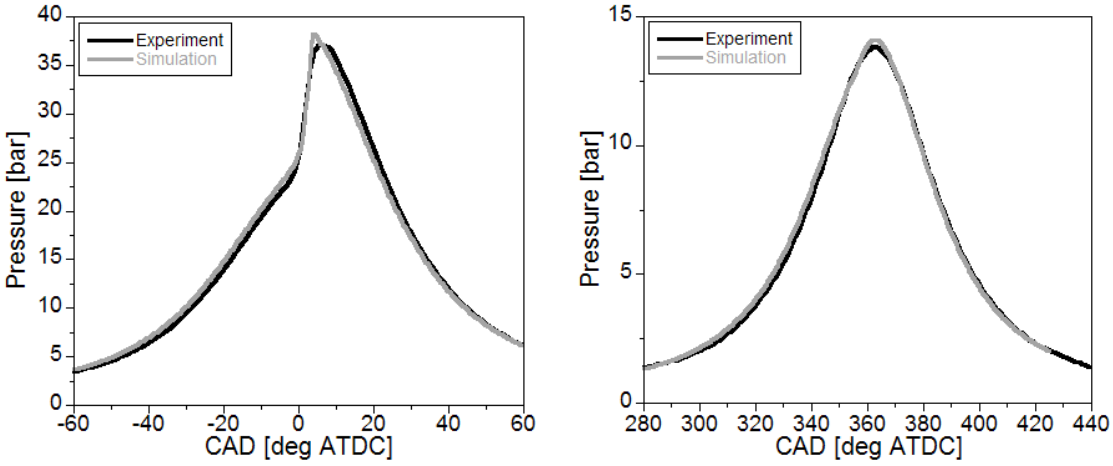
Six tables were required for the optimisation. This included an SI table, a table for the first NVO, transient valve timing NVO, transient valve timing HCCI and steady valve timing HCCI and NVO. The first table required in the transition is an SI table. The input parameters to the table were required to cope with changes in fuel mass, and spark timing as these parameters can be used to control the transition and hence can be optimised. As the opening of the throttle can affect the final SI cycle it was necessary to include the temperature and pressure at IVC as well. The EGR mass was assumed to remain constant.

Separate tables for transient NVO and the first NVO were produced due to the difference in exhaust gas composition from SI and HCCI combustion. Although named the first NVO table, it was also used in some cylinders for the 2^{nd} NVO due to large amounts of flame propagation in the first HCCI cycle. The fuel mass and injection timing were taken as control inputs that could be optimised. The temperature and pressure were required to cope with fluctuations due to the previous combustions and the changing valve phasing. The equivalence ratio was used as a fifth input to provide a composition at EVC, important due to the effect of NVO O_2 mass on the NVO heat release. The transient NVO table was similar to the 1^{st} NVO table apart from the O_2 mass fraction being used as an input instead of the equivalence ratio. Steady state NVO did not require the EVC pressure as it was used for NVOs after the valve phasing has finished. The four parameters chosen for this table were the same as the other transient NVO parameters.

The transient HCCI table needed to include fuel mass and spark timing for the same reasons as the SI table, and also the IVC temperature and pressure. As the EVC phasing is advanced during the transition, the EGR mass was also chosen as an input. As this was already 5 parameters it was not possible to include anything to give an EGR composition so this remained constant and was taken from the 2^{nd} NVO in cylinder 4 from a full SI-HCCI transition simulation.

For the steady state HCCI it was possible to remove the IVC pressure due to the table being used after the inlet manifold pressure has stabilized and the cam phasing has finished. EGR mass was assumed to remain constant. The spark timing was also no longer required due to it having little to no effect on HCCI combustion. The IVC temperature and fuel mass were then chosen as inputs along with the NVO heat release and NVO fuel mass. The NVO parameters were used to obtain an EGR composition. This was done by using the output compositions from the NVO table simulations. At each fuel mass, every component mass fraction was fitted to a cubic function of the NVO heat release. The fit was remarkably good and allowed the HCCI table to take into account how degraded the fuel injected during NVO was.

A similar approach could be taken for modelling the transition from HCCI to SI. This would require slightly different tables, notably the initial NVO table would not be needed and an initial SI table rather than an initial HCCI table would be required. This would need to account for the varying EGR mass in the first SI cycle and the composition of the



(a) Main combustion.

(b) NVO.

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

EGR. The necessary temperature and pressure ranges in the tables would also be different. The focus of this paper however is the transition from SI to HCCI.

4 Model Calibration

The tables were coupled with GT-Power, a one dimensional engine simulation tool, to enable multi-cycle, multi-cylinder simulation. GT-Power was used to model heat and mass flow through the engine during the intake and exhaust events. User models for the valve lift and throttle angle were required to simulate the transition from SI to HCCI.

The model was calibrated in HCCI and SI operating modes on the same GT-Power engine map. This was a difficult task and required a lot of tuning to make sure the IVC pressures and temperatures were adequate when the valve and throttle changes were made. To satisfy both HCCI and SI mode inlet temperatures as well as obtaining the correct pressures at IVC and also EVC during HCCI resulted in a well calibrated engine map. The wall temperature and heat transfer coefficients were set the same in both HCCI and SI to prevent further complications in the tabulation. Due to the speed of the transition and the large heat capacity of the engine block, this assumption was seen as acceptable for the initial HCCI cycles that were the focus of this work.

The model was calibrated at the speed and load of the transition in HCCI and SI modes by running 20 cycles with the steady state tables to reach equilibrium in both modes. The valve and throttle discharge coefficients were tuned to match the in-cylinder IVC and inlet manifold pressures at steady state in both modes. The wall temperatures were tuned to obtain the correct combustion phasing and fuel air equivalence ratios. The pressure profiles in Figure 2, show a good agreement between simulation and experimental measurements in HCCI mode. The EGR ratio was 48.4 % and 51.7 % in the simulation and experiment

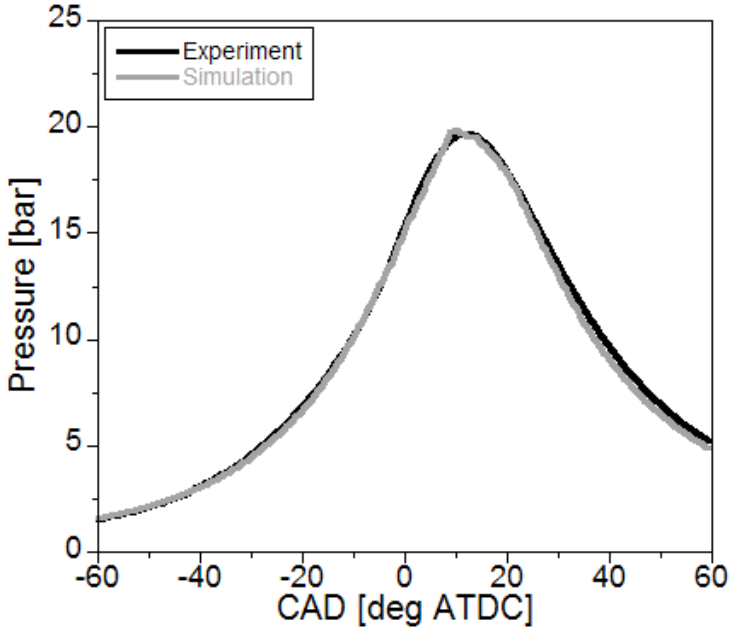


Figure 3: *Comparison of experimental and simulated steady state SI pressure profiles.*

respectively. The equivalence ratio was 0.71 in both the simulation and experiment. As this is highly dependent on the temperature, pressure, fuel mass and EGR mass, it suggests good temperature and pressure predictions at EVC and IVC. Figure 3 compares the steady state SI simulation result from the table coupled with GT-Power to an SI cycle with an average peak pressure and a good agreement was achieved.

5 Results

5.1 SI-HCCI Transition

The results of the SI-HCCI transition from the experiment and the fully tabulated SRM are compared in Figure 4. The results are all from cylinder 4 as the EGR ratio and equivalence ratio was measured in this cylinder. Figures 4a and 4b show the in-cylinder combustion pressure traces during the transition measured in the experiment and simulated with the model respectively. The trends in the pressure traces are well captured by the tabulated transition. The peak pressures in HCCI cycles 2 and 3 are slightly high, however this was seen as a good fit due to the complexity of the transition and the assumptions made in the tabulation. The constant EGR composition used in the transient HCCI cycles is likely to be a major source for the deviations from the experiment.

The NVO pressure traces from the experiment and simulation are shown in Figures 4c and 4d respectively. The tabulated peak pressures are slightly lower than those in the experiment, however when steady HCCI is reached the NVO traces match the experiment

well as was seen in Figure 2b.

Figure 4e compares the cylinder 4 equivalence ratios in the experiment and simulation during the transition. The model results match the experiment well, with only cycle 13, the third HCCI cycle, being slightly richer than the experimental measurement. This suggests the IVC temperature in the cycle was slightly high, which also caused the high peak pressure in the cycle as was seen in Figure 4b. This could be due to too much NVO heat release in the previous cycle as can be seen from Figures 4c and 4d the 2^{nd} NVO peak pressure trace was close to the 3^{rd} NVO's, when in the experiment the value was lower.

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. The calculation 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. A more detailed discussion of this transition is given in [21].

5.2 Optimisation

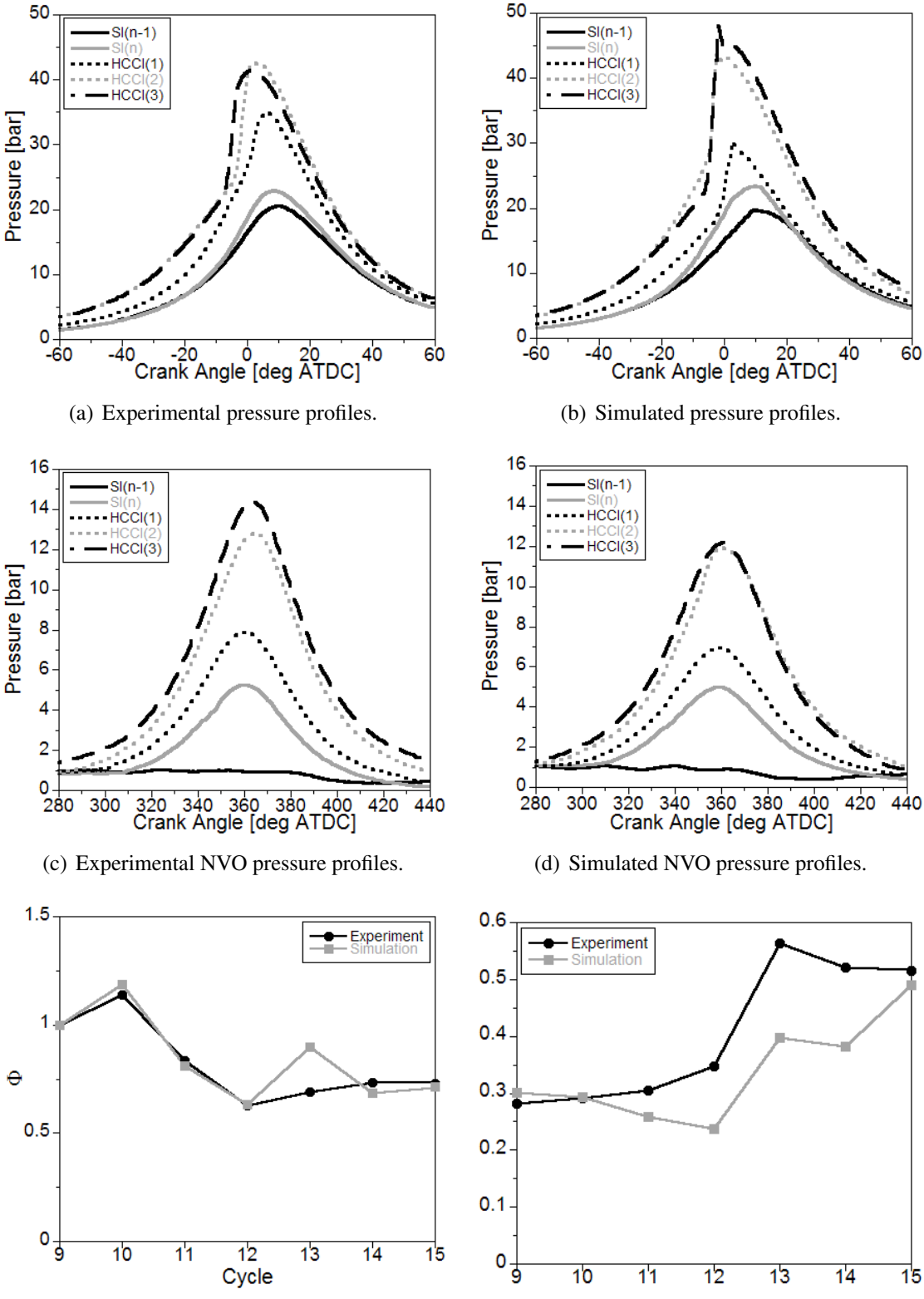
The GT-Power map was coupled with Simulink so that the MATLAB Optimisation Toolbox could be used and the transition called as a function. The optimisation function fmincon was selected to optimise the transition from SI-HCCI. The medium scale method is used, which uses a mixture of sequential quadratic programming, quasi-Newton and line search. The problem was set up to optimise 7 input parameters that can be controlled experimentally during the transition. These were; SI fuel mass f_{SI}, HCCI fuel mass f_{HCCI}, NVO fuel mass f_{NVO}, SI spark timing θ_{SIsp}, HCCI spark timing θ_{HCCIsp}, NVO injection timing θ_{NVOInj} and throttle command angle θ_{thr}.

A cost function was created with the aim of minimising IMEP fluctuations and also NO_x emissions. The IMEP cost was taken as the sum of the root mean square difference between each cylinder's IMEP and the target value of 2.6 bar. This was done over the first four transient cycles; the final SI cycle and the three consecutive HCCI cycles. The cost was weighted so that the third HCCI cycle's IMEP had more influence than the previous cycles, as described in Equation (1), in order to produce a more stable transition.

$$\begin{aligned}\text{IMEPCost} =& 0.2 \times (\text{IMEPCost}_{SIn} + \text{IMEPCost}_{HCCI1} + \text{IMEPCost}_{HCCI2}) \\ &+ 0.4 \times \text{IMEPCost}_{HCCI3}\end{aligned} \tag{1}$$

It was found in [21] that the NO_x emissions in the first HCCI cycle are extremely large, so the sum of the NO_x emissions from each cylinder in the last SI and first two HCCI cycles was taken as the second cost, NO_xCost. The values obtained from the previous calibration run were used to normalize the values, making both costs equal to unity for the previous transition. As the IMEP cost is seen as more important and more difficult to minimise it was given a 90 % weighting and the NO_x cost was given a 10 % weighting as described in Equation (2).

$$\text{TotalCost} = 0.9 \times \text{IMEPCost} + 0.1 \times \text{NO}_x\text{Cost} \tag{2}$$



(a) Experimental pressure profiles.

(b) Simulated pressure profiles.

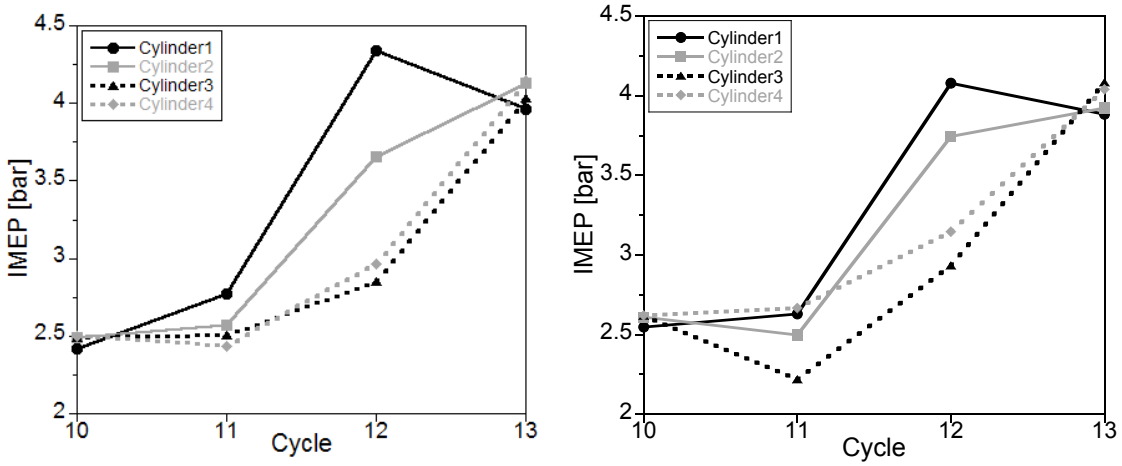
(c) Experimental NVO pressure profiles.

(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.*



(a) Initial values.

(b) Optimised values.

Figure 5: *IMEP during transition using initial control parameters and optimised parameters.*

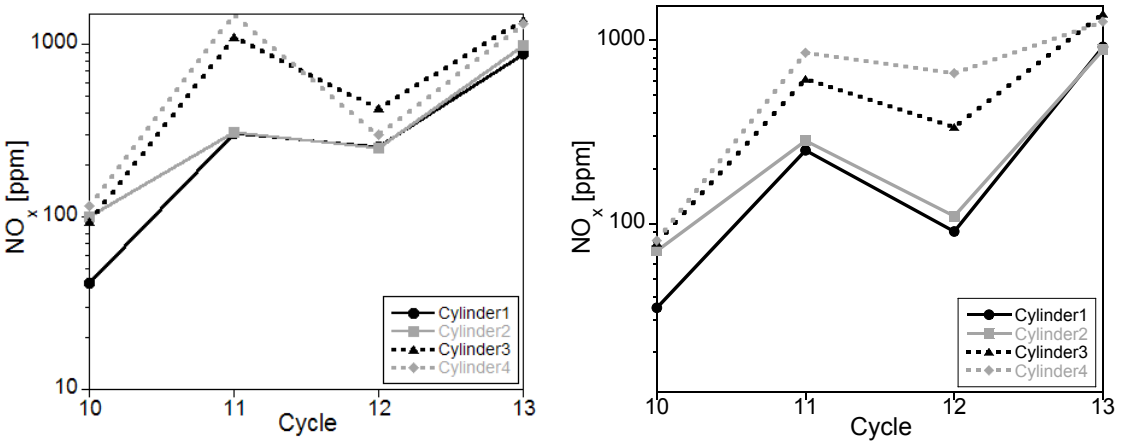
The control parameter limits that were used and initial values are given in Table 3. The optimisation finished in 34.5 hours and after 553 transition evaluations on a 2.21 GHZ Athlon X2 with 2.00 GB of RAM. The cost function for IMEP reduced from 1 to 0.98 and the NO_x cost function reduced from 1 to 0.66 giving a final cost of 0.95. Table 3 shows the transition input parameters before and after the optimisation.

Table 3: *SI-HCCI control parameters limits and values before and after optimisation.*

Parameter	f_{SI}	f_{HCCI}	f_{NVO}	θ_{SIsp}	θ_{HCCIsp}	θ_{NVOInj}	θ_{thr}
Min.	8.5 mg	4.5 mg	1.6 mg	-60 CAD	-60 CAD	285 CAD	1 CAD
Max.	11.5 mg	7.0 mg	3.4 mg	-40 CAD	-30 CAD	360 CAD	720 CAD
Before Opt.	11.3 mg	6.6 mg	1.7 mg	-55 CAD	-60 CAD	360 CAD	1 CAD
After Opt.	11.5 mg	6.1 mg	1.6 mg	-43 CAD	-55 CAD	360 CAD	1 CAD

Figure 5 compares the tabulated transition's IMEP in the first 4 transition cycles, before and after the optimisation. The overall results are closer to the 2.6 bar target, although results for all cylinders in the 3^{rd} HCCI cycle, cycle 13, and for cylinders 1 and 2 in the twelfth cycle, are still a lot higher than desired. After cycle 13 the deviations were greatly reduced and stable HCCI combustion was achieved in all cylinders. The high IMEP in the final transient cycles could be due to the constant EGR composition used in the transient HCCI cycles. The EGR composition was kept constant due to the limit in the number of input parameters for the table. The composition may have prevented the optimisation from reducing the IMEP any further. The limit in the tables' input parameters is the main disadvantage in the tabulation technique when it comes to simulating such a complex process.

Figure 6 compares the initial NO_x concentrations during the tabulated transition with



(a) Initial values.

(b) Optimised values.

Figure 6: *NO_x emissions during transition using initial control parameters and optimised parameters.*

those from the optimised transition. It can be seen that the overall NO_x emissions in cycles 11 and 12 have been reduced by the optimisation. This was achieved through reductions in fuel mass during the transition, resulting in lower peak combustion temperatures.

The spark timing was retarded in both the final SI cycle and the first HCCI cycles. This delays the combustion phasing and reduces the peak cylinder temperatures, lowering NO_x emissions and reducing the IMEP during the transition. The fuel mass in the first HCCI cycles was reduced for the same reason. The NVO fuel mass was reduced and injection timing kept at the most retarded timing to reduce NVO heat release, reducing the IVC temperatures. The throttle was opened slightly later. The change from the initial control values was not great. The initial values were chosen through a manual optimisation and the transition was quite stable, making it difficult for the optimisation to improve on.

6 Conclusions

A stochastic reactor model (SRM) was used to simulate the complex transition from SI to HCCI. A good agreement between the model and experimental results was obtained. The detailed chemistry model was then tabulated to allow fast simulation of the transition. The tabulated transition was achieved by creating 6 different tables, each used for simulating a different part of the transition. Tables for the first NVO, transient valve timing NVO, transient valve timing HCCI, steady valve timing HCCI and NVO and SI combustion were required.

The tables were calibrated by simulating steady state SI and HCCI before the transition was simulated. The pressure profiles from the tabulated SRM matched experimental data well in both steady state and during the transition. During the transition experiment the EGR ratio and equivalence ratio were measured in cylinder 4, the second cycle to transition, and the tabulated transition made a good prediction of the results.

The tabulated transition was optimised using the MATLAB function fmincon. The model allowed fast simulation of the transition with emissions prediction. This enabled a cost function to be setup to penalise any deviations from the steady state IMEP and also any NO_x emissions. The optimisation took 34.5 hours and resulted in a smoother transition and reduced NO_x. The technique will be used for experiment design and could also be used for investigating engine controllers before conducting more costly experiments. One of the main advantages of the technique over using a Wiebe function for fast simulation is the emissions prediction capability.

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Abbreviations

ATDC	After top dead centre
CAD	Crank angle degree
EGR	Exhaust gas recycle
EMST	Euclidean minimum spanning tree
EVC	Exhaust valve close
EVO	Exhaust valve open
GDI	Gasoline direct injection
HCCI	Homogeneous charge compression ignition
IMEP	Indicated mean effective pressure
IVC	Inlet valve close
IVO	Inlet valve open
NDIR	Non-dispersive infrared
NVO	Negative valve overlap
PDF	Probability density function
PRF	Primary reference fuel
RAM	Random access memory
RON	Research octane number
SI	Spark ignition
SRM	Stochastic reactor model
TDC	Top dead centre
UEGO	Universal exhaust gas oxygen

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