

A Detailed Chemistry Multi-cycle Simulation of a Gasoline Fueled HCCI Engine Operated with NVO

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ABSTRACT

A previously developed Stochastic Reactor Model (SRM) is used to simulate combustion in a four cylinder in-line four-stroke naturally aspirated direct injection Spark Ignition (SI) engine modified to run in Homogeneous Charge Compression Ignition (HCCI) mode with a Negative Valve Overlap (NVO). A portion of the fuel is injected during NVO to increase the cylinder temperature and enable HCCI combustion at a compression ratio of 12:1. The model is coupled with GT-Power, a one-dimensional engine simulation tool used for the open valve portion of the engine cycle. The SRM is used to model in-cylinder mixing, heat transfer and chemistry during the NVO and main combustion. Direct injection is simulated during NVO in order to predict heat release and internal Exhaust Gas Recycle (EGR) composition and mass. The NO_x emissions and simulated pressure profiles match experimental data well, including the cyclic fluctuations. The model predicts combustion characteristics at different fuel split ratios and injection timings. The effect of fuel reforming on ignition timing is investigated along with the causes of cycle to cycle variations and unstable operation. A detailed flux analysis during NVO unearths interesting results regarding the effect of NO_x on ignition timing compared with its effect during the main combustion.

INTRODUCTION

The widespread use of Internal Combustion Engines (ICE) and growing concerns over climate change have made it necessary to improve the efficiency and emissions of modern engines. HCCI has shown potential as an alternate ICE operating mode that offers low NO_x and particulate emissions and high efficiency. Unlike SI and Compression Ignition Direct Injection (CIDI) engines, in which combustion is initiated with a spark or fuel injection, there is no direct ignition control in HCCI. The in-cylinder temperature, pressure and composition at Inlet Valve Closing (IVC), and to a lesser extent the turbulence, determine the combustion phasing, making HCCI more difficult to control than conventional operating modes. To accurately model HCCI combustion it is therefore beneficial to use a detailed chemical mechanism. Probability Density Function (PDF) based models have proven advantageous for simulating HCCI combustion due to their ability to incorporate detailed chemistry whilst maintaining low computational times [1].

Several different strategies for achieving stable HCCI have been investigated including; heating the intake air [2], boosting the intake pressure [3], varying the compression ratio [4] and the use of dual fuels or fuel additives [5]. The application of alternative fuels, such as n-butane, propane, ethanol etc., has also been explored [3].

There are still problems with HCCI operation. Due to the low combustion temperatures, HCCI operation can produce high CO and unburned hydrocarbon (UHC) emissions. Currently HCCI can only be used within a

narrow operating range. The low load limit occurs when the fuel concentration is too low to be ignited properly causing unstable operation. During startup the charge is too cold for HCCI operation. At high loads the large rates of heat release lead to engine knock.

A possible solution is to switch back to a conventional mode of operation at certain loads. The transition from SI or CIDI to HCCI is challenging due to the different temperatures and exhaust gas composition in each of the modes of operation [6-7]. Switching from HCCI to another mode is less problematic, however it is still important to obtain a smooth transition [8].

To achieve HCCI combustion at compression ratios used in SI engines a NVO can be used to trap exhaust gas in the cylinder, and utilize its thermal energy to raise the IVC temperature [9-10]. It also dilutes the charge, reducing the rate of heat release, making it possible for higher loads to be achieved without knock. EGR increases the heat capacity of the charge, which reduces the effect of air temperature on combustion [11] and reduces the peak combustion temperature, helping to prevent NO_x formation [12]. The use of internal EGR causes each cycle to rely on the temperature and exhaust gas composition of the previous cycle. It was found that oscillatory cycles can occur when a late combustion is quenched, causing a large amount of UHC to be present in the residual gas which burns during NVO advancing the following cycle's combustion phasing [10].

Certain exhaust species retained by EGR may have a large influence on the combustion in the following cycle. At high EGR ratios, combustion duration may be shortened by CO₂ and H₂O [13]. It has also been suggested that H₂O advances ignition timing by a chemical effect [12]. It was found that low concentrations of NO caused combustion phasing to advance [14-15]. It was suggested that NO advances combustion by the production of the reactive OH radical as shown in Reaction (1).



The use of direct injection (DI) enables the amount and timing of fuel injection to be varied as well as allowing multiple injections per cycle. Injecting a fraction of the fuel during NVO and the remainder during intake is a promising strategy for controlling HCCI. This has been found to increase the lean limit and reduce fuel consumption [16]. It produces a nearly homogeneous mixture which results in an efficient, stable and fast combustion [17]. The early injection can also result in reduced NO_x and UHC emissions for the same reason [18]. Injecting during NVO can increase pumping losses from the drop in cylinder temperature and pressure as the fuel evaporates [19]. The opposite effect can be

observed when heat is released during the NVO expansion [18]. The reactions that take place have also been reported to increase the fuel's ignitability and advance the combustion phasing [20-22]. This effect is known as fuel reforming and can expand the lean limit of combustion without increasing NO_x emissions [16]. Advancing the NVO injection timing or increasing the fraction of fuel injected can advance the main combustion phasing due to increased NVO heat release and fuel reforming [20-22]. The magnitude of control these strategies offer is however highly dependent on the amount of O₂ available during NVO [23].

Simulations can be used to gain further insight into the complex processes occurring in HCCI engines and may be used for optimizing control [24]. When a large amount of EGR is used, multi-cycle simulations are required to couple consecutive cycles. PDF based models can be used with detailed chemistry at relatively low computational cost making them a useful tool for multi-cycle engine simulation.

The paper is structured as follows. Details of the model are described in the next section. The following section shows results from the calibrated model. Simulation and experimental results are then compared at various split ratios and injection timings. Next an investigation into the causes of cycle to cycle variations (CCV) and unstable operating conditions is presented. The effect of fuel reforming is then discussed and some interesting results regarding the effect of NO_x on combustion phasing are shown. Conclusions are drawn in the final section.

MODEL DETAILS

The previously developed Stochastic Reactor Model (SRM) [1,25,26] has been used to simulate an HCCI engine operated with a 146 CAD NVO. The model is based on the PDF transport equation [27] and uses the Euclidean Minimum Spanning Tree (EMST) mixing model [28]. The model also contains stochastic heat transfer and direct injection sub-models. A detailed Primary Reference Fuel (PRF) chemical mechanism containing 157 species and 1552 reactions was used.

Details of the engine are given in Table 1. A split injection strategy was used, in which 20-40 % of the fuel was injected during NVO, referred to as pilot injection. The pilot injection timing was also varied. The second injection took place during the intake stroke and was assumed to result in a homogenous mixture at IVC. For this reason all particles at IVC were given the same composition and temperature. The cooling effect of spray evaporation was accounted for at IVC. The compositions at IVO and EVO were stored and used as the EGR composition at the following closed valve

event. The mass and composition of EGR at IVO was also stored and used as the mass and composition of EGR at IVC. It was assumed that any EGR lost through the intake valve is re-inducted during the next intake stroke and that the difference in its composition and mass between consecutive cycles is small enough to cause no effect. Due to fluctuations in air and EGR mass in each cycle, the fuel mass rather than equivalence ratio was set and the EGR mass instead of ratio was used. 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. Each case was run for 40 cycles with 100 stochastic particles.

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
CR	12.0
IVO [CAD BTDC]	295
IVC [CAD BTDC]	125
EVO [CAD ATDC]	109
EVC [CAD ATDC]	279
Start of main inj. [CAD BTDC]	260

MODEL CALIBRATION

The different operating conditions modelled are given in Table 2. The base case, case 1, was used to calibrate the engine model parameters. Cases 2 and 3 had different fuel split ratios compared to the base case. The fuel split ratio is the mass of fuel supplied in the main injection divided by the total amount used per cycle. Cases 4 and 5 had different pilot injection timings to the base case.

Table 2: Engine operating conditions.

Case	1	2	3	4	5
Fuel split	0.8	0.7	0.6	0.8	0.8
Pil. inj.[CAD ATDC]	315	315	315	305	285
Fuel [mg/cyl/cyc]	9.77	9.85	9.90	9.75	9.78
λ	1.33	1.32	1.31	1.32	1.29
Speed [RPM]	1511	1511	1511	1510	1513
BMEP [bar]	2.62	2.61	2.61	2.60	2.59

Figure 1 shows the average pressure profiles during the main combustion of case 1 for 40 simulated and 200 experimental cycles. The simulation matches experimental data well. The NVO pressure profiles are compared in Figure 2 and suggest the simulated heat release during NVO is slightly lower and occurs later than it does in the experiment. Peak pressures against the crank angle they occurred for forty consecutive cycles are compared with experimental results in Figure 3. Peak pressures occur slightly earlier in the simulation than the experiment. The average fuel air equivalence ratio obtained in the simulation was 1.25, compared with a measured value of 1.33. This value is important as a poor match would suggest incorrect EGR mass and temperatures at IVC and EVC. Emissions data is given in Table 3. The NO_x result suggests temperatures in the simulation were a good match to the experiment. The model contains a crevice but no wall impingement sub-model, which could be one cause of the low UHC and CO emissions obtained in the simulation. The engine was also operated in SI mode at the same speed and load with an injection timing of 308 CAD BTDC, producing 3120 ppm UHC and 4900 ppm CO. These are very close to the HCCI values suggesting that wall impingement could be a major cause of UHC and CO in the engine. The UHC emissions should not have a direct impact on the following combustion due to the fuel injected during NVO, however the NVO heat release may be effected. Consecutive cycles did not appear to show a trend as can be seen by comparing peak pressures in Figure 4. This result agreed with the experimental data.

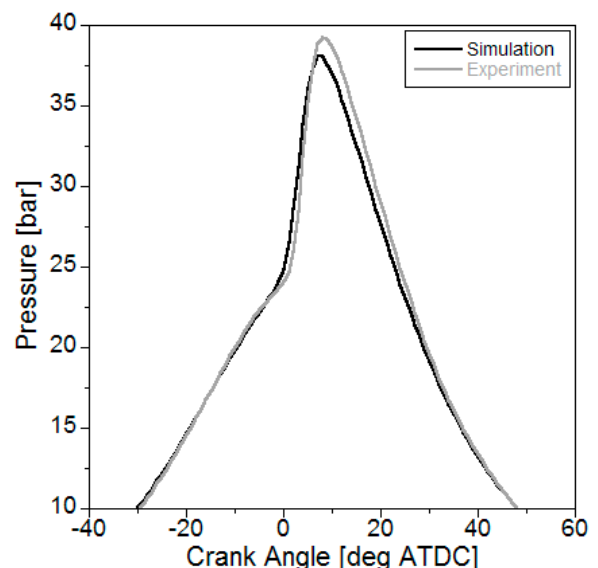


Figure 1: Average pressure profile during main combustion of 40 simulated and 200 experimental cycles of case 1.

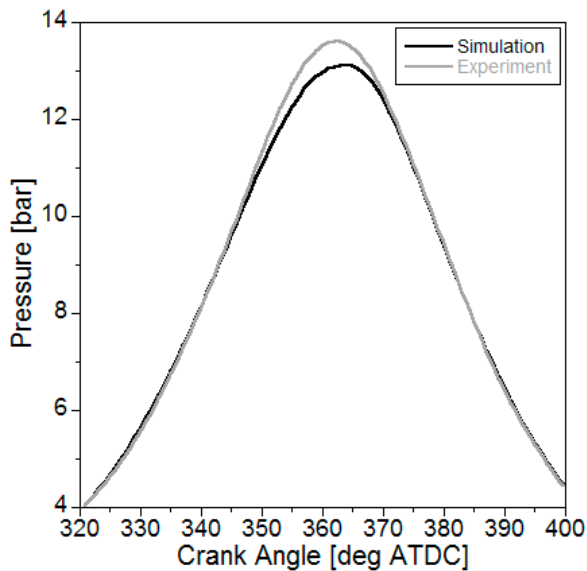


Figure 2: Average pressure profile during NVO of 40 simulated and 200 experimental cycles of case 1.

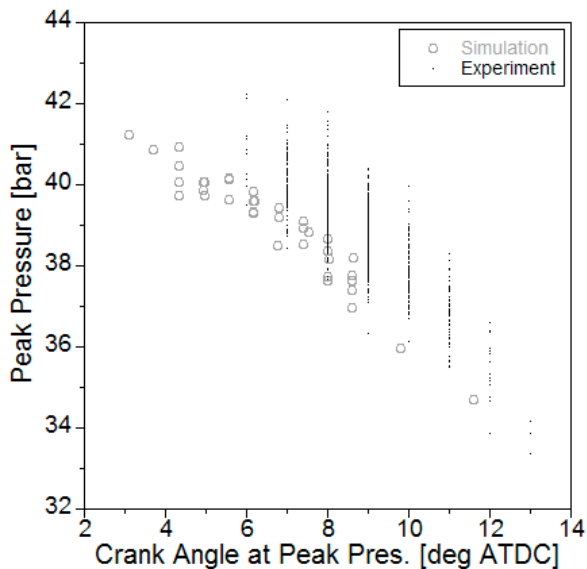


Figure 3: Peak pressure against the crank angle it occurs for 40 simulated and 200 experimental cycles of case 1.

Table 3: Average emissions over 200 experimental and 40 simulated cycles (33 cycles for case 3).

Specie	Cas	1	2	3	4	5
NOx [ppm]	Exp.	15.2	20.5	24.7	14.3	16.9
	Sim.	8.0	9.9	10.9	8.0	7.8
CO [ppm]	Exp.	103	1008	1029	964	956
	Sim.	13.1	244.3	115.2	281.2	89.4
UHC [ppm]	Exp.	295	2789	2604	2924	297
	Sim.	8.5	57.2	30.5	65.2	22.1

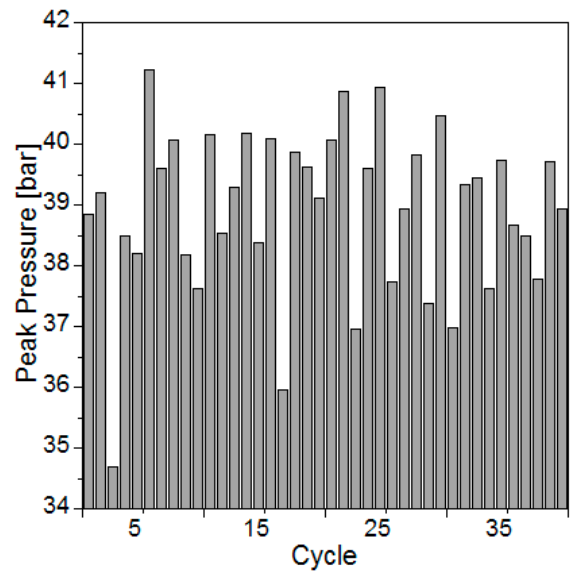


Figure 4: Peak pressure against the cycle it occurs for 40 simulated cycles of case 1.

FUEL SPLIT

The fuel split ratio was varied in cases 1-3 as shown in Table 2 with the other parameters the same as in Table 1. All model parameters used were kept constant apart from the values given in Table 2, which were varied in the experiments. Figure 5 shows a decrease in the fuel split ratio caused an advance in combustion phasing. The same trend was seen in the simulation as shown in Figure 6. The average peak pressure was however lower with lower fuel split ratios, which did not occur in the experiment. This was probably due to a larger variation in combustion phasing in the simulations and the effect of averaging the pressure profiles.

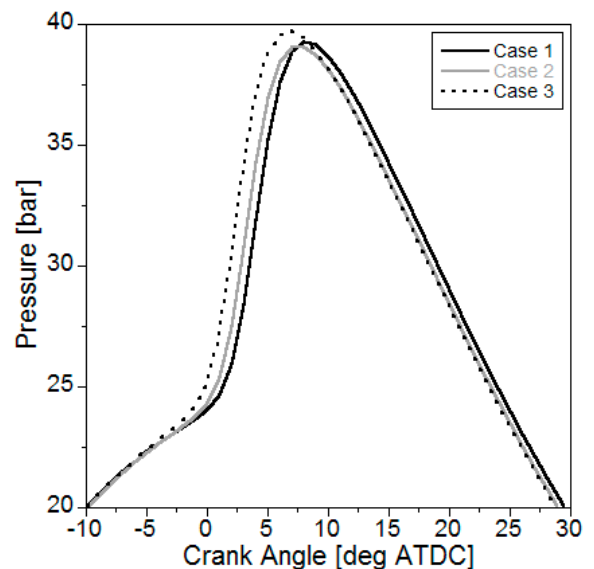


Figure 5: Average experimental combustion pressure profiles over 200 cycles for cases 1-3.

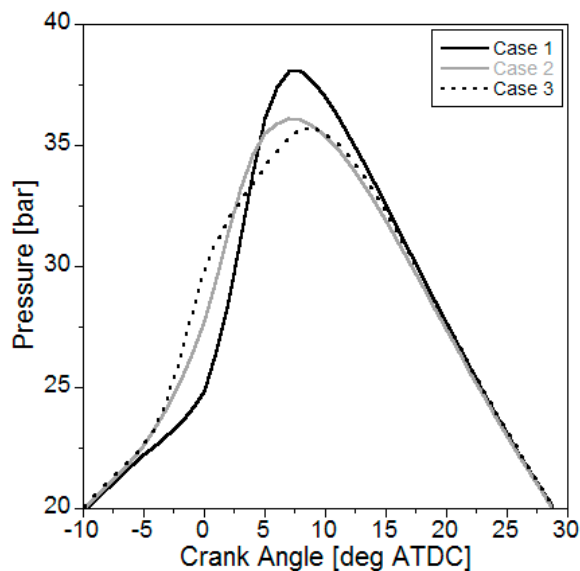


Figure 6: Average simulated combustion pressure profiles over 40 cycles for cases 1 and 2 and 33 cycles for case 3.

Table 4: Average results over 40 cycles (33 cycles for case 3).

Case	1	2	3	4	5
Lambda	1.25	1.24	1.23	1.25	1.25
Lambda NVO	1.02	0.93	0.85	1.02	1.02
IVC T [K]	503.5	503.9	502.8	504.3	506.1
EVC T [K]	695.0	697.5	697.3	695.9	694.4
NVO heat rel. [J]	43.1	43.5	42.7	43.6	45.2
CA50 [deg ATDC]	3.6	3.5	3.3	4.1	2.9
Internal EGR [%]	48.2	48.1	48.0	48.2	48.1

The advance in combustion phasing has been reported in the literature as due to increased NVO heat release and due to the fuel becoming more reactive from reactions during NVO. The average IVC temperatures in cases 1-3 are given in Table 4 and show only a slight variation as does the NVO heat release. This suggests the reason for advanced combustion phasing is the fuel reforming effect. The NO_x emissions increased as more fuel was injected during NVO, matching the experimental trend. This is probably due to combustion occurring closer to TDC resulting in higher temperatures. By comparing Tables 4 and 2, it can be seen that the air fuel equivalence ratio decreased with a decrease in fuel split ratio, which was also observed in the experiment. Figures 7 and 8 show the NVO pressure profiles in the experiment and simulation for the three cases. The pressure before TDC is lower when the fuel mass injected during NVO is increased. This was due to the evaporation of the fuel cooling the charge. The effect of varying fuel split ratio is investigated further in the Fuel Reforming section.

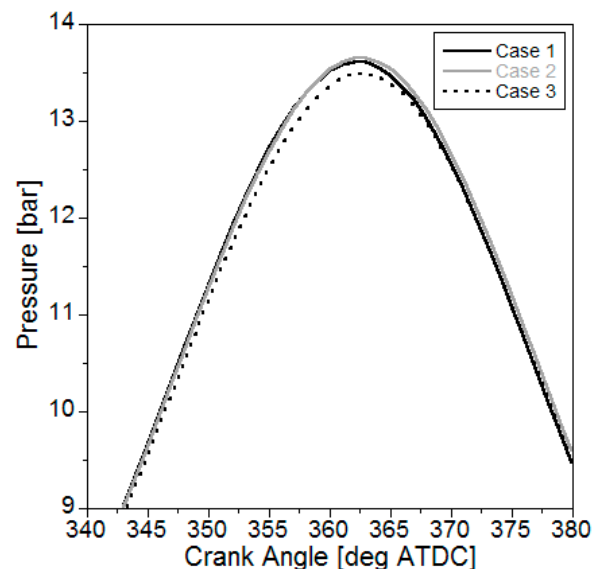


Figure 7: Average experimental NVO pressure profiles over 200 cycles for cases 1-3.

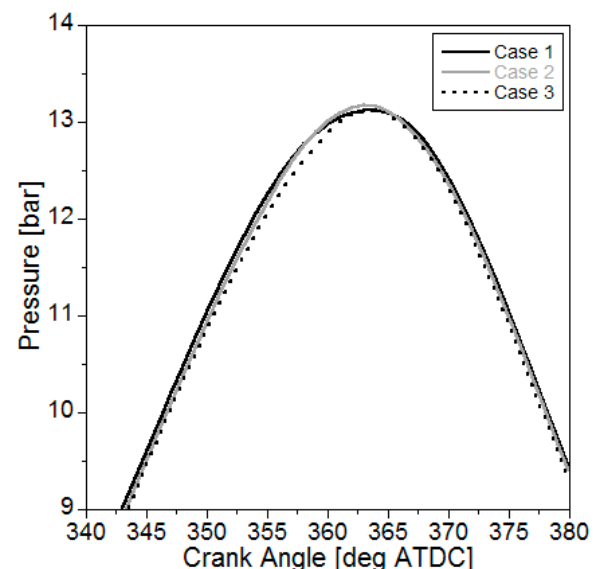


Figure 8: Average simulated NVO pressure profiles over 40 cycles for cases 1 and 2 and 33 cycles for case 3.

The average pressure profiles and values for case 3 are only for the first 33 cycles as a misfire occurred in cycle 34. This will be discussed in the Cyclic Variation and Instabilities section.

INJECTION TIMING

The pilot injection timing was varied in cases 1, 4 and 5 as shown in Table 2 with the other parameters the same as in Table 1. All model parameters were kept constant