Cambridge Centre for Computational Chemical Engineering University of Cambridge

Department of Chemical Engineering

Preprint ISSN 1473 – 4273

Influence of Injection Timing and Piston Bowl Geometry on Diesel PCCI Combustion and Emissions

Li Cao [1] , Amit Bhave [1,2] , Haiyun Su [1] , Sebastian Mosbach [1] , Markus Kraft [1] , Antonis Dris [3] , Robert M. McDavid [3]

released: 23 January 2009

[1] Department of Chemical Engineering
University of Cambridge
New Museums Site
Pembroke Street
Cambridge, CB2 3RA
UK
E-mail: mk306@cam.ac.uk

[2] Reaction Engineering Solutions Ltd.
William Gates Building
JJ Thompson Avenue
Cambridge, CB3 0FD
UK

[3] Caterpillar Inc.
Engine Technologies Europe
Frank Perkins Parkway
Peterborough, PE1 5NA
UK

Preprint No. 65

c4e

Key words and phrases: early DI Diesel, Piston geometry, 3D CFD, Stochastic reactor model

Edited by
Cambridge Centre for Computational Chemical Engineering
Department of Chemical Engineering
University of Cambridge
Cambridge CB2 3RA
United Kingdom.

Fax: + 44 (0)1223 334796
E-Mail: c4e@cheng.cam.ac.uk
World Wide Web: http://www.cheng.cam.ac.uk/c4e/

Abstract

Premixed Charge Compression Ignition (PCCI), a Low Temperature Combustion (LTC) strategy for diesel engines is of increasing interest due to its potential to simultaneously reduce soot and NO_x emissions. However, the influence of mixture preparation on combustion phasing and heat release rate in LTC is not fully understood. In the present study, the influence of injection timing on mixture preparation, combustion and emissions in PCCI mode is investigated by experimental and computational methods. A sequential coupling approach of 3D CFD with a Stochastic Reactor Model (SRM) is used to simulate the PCCI engine. The SRM accounts for detailed chemical kinetics, convective heat transfer and turbulent micro-mixing. In this integrated approach, the temperature-equivalence ratio statistics obtained using KIVA 3V are mapped onto the stochastic particle ensemble used in the SRM. The coupling method proved to be advantageous in terms of computational expense and emission prediction capability, as compared with direct coupling of CFD and chemical kinetics. The results show that the fuel rich pockets in the late injection timing are desirable for triggering auto-ignition and advancing the combustion phasing. Furthermore, the model is utilised to study the impact of combustion chamber design (open bowl, vertical side wall bowl and re-entry bowl) on PCCI combustion and emissions. The piston bowl geometry was observed to influence the in-cylinder mixing and the pollutant formation for the conditions studied.

Contents

1 Introduction

Low Temperature Combustion (LTC) modes such as Homogeneous or Premixed Charge Compression Ignition (HCCI/PCCI) are receiving increased attention due to their potential for simultaneously reducing soot and NOx emissions from Direct Injection (DI) diesel engines. PCCI mode involves premixed combustion of a highly diluted or lean mixture and the combustion process is primarily controlled by the chemical kinetics. Thus, the control of ignition timing and burning rate in PCCI combustion is fundamentally more challenging than in a conventional compression ignition DI diesel engine governed mainly by physical processes such as fuel-air mixing. Furthermore, for the cases where the air-fuel charge is often not purely homogeneous, the influence of fuel-air mixing on combustion also needs to be taken into account. In addition to experimental studies, a variety of computational modelling approaches based on multi-dimensional computational fluid dynamics (CFD) have also been applied to investigate early direct injection PCCI combustion. The detailed chemical kinetics and the flow description in PCCI mode are relatively decoupled, when compared to conventional diesel combustion. This fact has been exploited by sequential solvers based on CFD and multi-zone combustion models [1, 3, 11]. In a multi-zone approach, the computational cells having similar temperature and composition histories are grouped into a relatively small number of zones (about 10). The chemical kinetics solver is applied to each zone, assumed as a well stirred reactor. Flowers et al. [11] modified the multi-zone model to include mixing effects, by mapping the temperature distributions from CFD to the individual zones throughout the cycle. Babajimopoulos et al. [4] further improved the approach by with a two-way coupling between the CFD cells and the zones based on the thermodynamic and chemical properties at each computational time step. Several assumptions were made in order to re-distribute the species from the zones to the CFD cells while ensuring that the properties (composition of each species) are conserved. Firstly the mass of each cell and each individual species in the zone must be conserved. Secondly, the number of C, H, O and N atoms in each cell must be conserved. In the most extreme case, the direct integration of CFD with detailed chemistry involves the use of detailed kinetics to solve the chemistry within each computational cell in the CFD domain [15].

The aforementioned methods rely on the assumption that the variations in the scalar variables (temperature and equivalence ratio) are negligible within each zone or computational cell, when turbulence/chemistry interactions are weak. However, the presence of significant stratification during late fuel injection and the need for accurate emission predictions require the explicit accounting for turbulence and chemistry interaction. A more direct and detailed representation of the complex interactions occurring in small length scales between turbulence and kinetics can be achieved by implementing a more advanced turbulent combustion model. Zhang et al. [29] used a joint PDF containing 40 chemical species and mixture enthalpy to model HCCI combustion. Their results demonstrate the importance of accounting for turbulence-chemistry interactions with increasing stratification. Alternative approaches, mostly variants comprising of the Shell ignition model

and Characteristic Time Combustion (CTC) approach in KIVA 3V have also been applied to early DI diesel engine studies [16]. In particular, Jhavar et al. [14] highlighted that the in-cylinder temperature distribution at the end of the fuel injection event was a major contributor to the ignition dwell duration and that the air-fuel distribution affected the ignition dwell to a smaller extent. Recently, the coefficient of turbulent time scale, f, within the CTC model was correlated with non-uniformity (standard deviation of equivalence ratio) to study the influence of multiple injections on in-cylinder pressure in PCCI mode [17, 28]. Furthermore, Diesel fuelled PCCI combustion was also studied by Kong et al. [18] comparing the KIVA /RIF (Representative Interactive Flamelet) approach with a direct integration of kinetics and CFD. The RIF approach employed a single flamelet and accounted for the effects of evaporation on turbulence-chemistry interaction. Elsewhere, the evaporation source term in the mixture fraction variance equation has been investigated by applying a transient interactive flamelet approach and a transient flamelet library based approach to simulate PCCI combustion in a medium duty Diesel engine [19]. Enthalpy-based flamelet model has also been developed to model auto-ignition with thermal inhomogeneities for HCCI application [10].

The present study focuses on the development of an integrated computational model for simulating direct injection diesel PCCI engine combustion and emissions at a reasonable computational cost, while being capable of capturing geometry related effects. A direct coupling of 3D CFD and detailed chemical kinetics is used from Intake Valve Closing (IVC) to account for fuel spray and mixing followed by the low temperature combustion process. Prior to the onset of high temperature combustion, the results are then used to initialize the notional particles in the probability density function (PDF)-based Stochastic Reactor Model (SRM) with detailed chemical kinetics. Consequently, the main combustion and expansion processes until the Exhaust Valve Opening (EVO) are then simulated using the SRM. The work presented here is the progression of the 2D CFD-SRM coupling based study applied to an early injection diesel engine at idle condition [8]]. The SRM approach has been previously applied as a stand-alone tool [20, 24] as well as coupled with 1-D engine cycle simulators [5, 26].

This paper is structured as follows: First, the diesel engine set-up under consideration is explained and the operating conditions are discussed. Then the methodology of sequential coupling of 3D CFD and SRM is described. This is followed by the description of the model validation against the measurements for combustion and emissions. Next, a parametric study of the influence of injection timing sweep on combustion characteristics and emissions (CO, HC and NO) is included. Furthermore, the effect of engine bowl geometry on mixture formation, PCCI combustion and emissions is investigated using the integrated simulation tool. Finally, the conclusions are drawn at the end.

2 Engine Set-up

Experimental data for validation of the combustion models was collected from a Caterpillar multi-cylinder test engine (MCTE). The base engine configuration is given in Table 1. A typical injection rate shape is given in Figure 1. Engine-out emissions data was collected from the engine during steady-state PCCI operation. Specifically, NO, unburned hydrocarbons (uHC) and CO were recorded. Additionally, direct filter paper soot measurements were made at selected points. High speed cylinder pressure data was also collected at multiple steady state operating points, however in this paper, only the results for one engine speed and load at different injection timings are presented. For combustion phasing, both external exhaust gas recirculation and Intake Valve Actuation (IVA) were used. Additionally, the IVA was employed to reduce cylinder-to-cylinder variation in combustion behaviour as indicated by alignment of apparent heat release rate from all six cylinders.

Table 1: *Capterpillar MCTE specification.*

Parameter	**Value**
Bore	137.1 mm
Stroke	171.5 mm
Conrod length	270.0 mm
Displacement (6 cyls)	15.2 L
Compression ratio	10:1
Engine speed	1200 rpm
Engine load	1029 Nm
BMEP	850 kPa
Nozzle hole size	0.129 mm
Injection pressure	170-190 MPa
Nominal AVL swirl	0.3

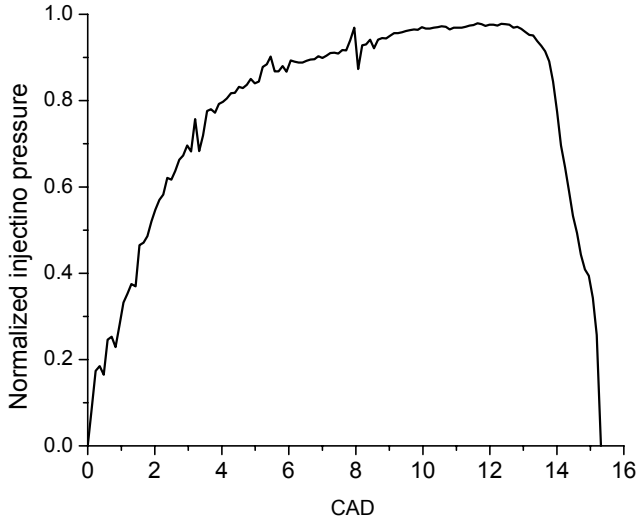


Figure 1: *Normalized injection rate profile for Caterpillar MCTE.*

3 Model Description and Validation

In this section, the coupling strategy of 3D CFD with SRM approach is discussed and the integrated model is validated against the measurements.

3.1 Direct coupling of CFD and detailed chemical kinetics

The CFD simulation was carried out using the KIVA3V code [2], with improvements in turbulence, gas/wall heat transfer, spray breakup and combustion models [13]. The RNG $k-\epsilon$ turbulence model [13] was used for the engine flow simulation; a hybrid wave aerodynamics breakup model, combining Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) [22] instability wave mechanisms, was applied to simulate high pressure spray atomization. The effects associated with spray/wall interactions including droplet splash and film spreading due to impingement forces were considered in a wall-film sub-model [21]. The physical properties of tetradecane were used to simulate the physics of diesel fuel, while a detailed n-heptane reaction mechanism, comprising of 157 chemical species and 1552 reactions [20] was used to simulate diesel fuel chemistry. An in-house chemistry interface was used for interpreting the kinetics mechanism and the chemical kinetics Ordinary Differential Equations (ODE) were integrated by the numerical solver (RADAU5) [12]. This chemistry interface was incorporated directly into KIVA 3V to solve the n-heptane re-

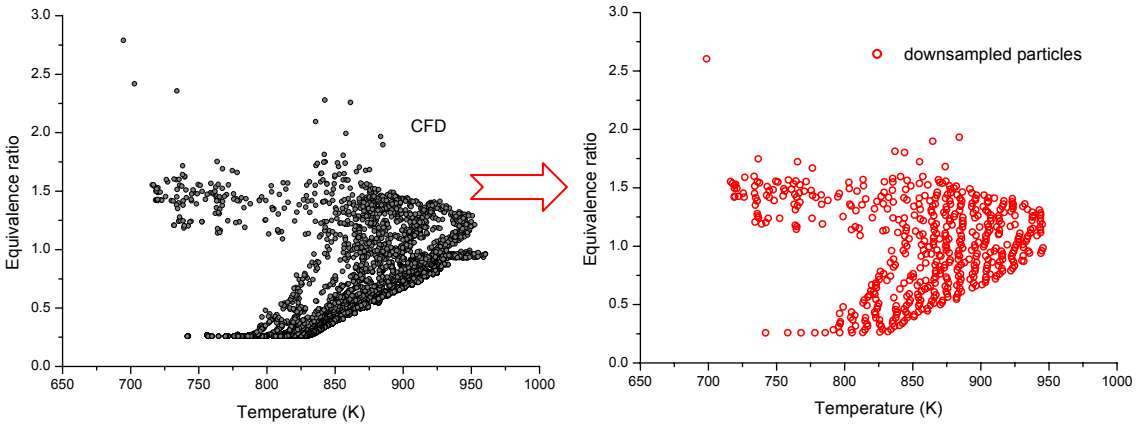
action mechanism during multidimensional engine simulations. Each computational cell was considered as a well stirred reactor. The authors are aware of the lack of the sub-grid turbulence-kinetics interaction and future work will focus on a new closure model. In this study KIVA 3V was used to solve the low temperature chemistry only.

3.2 Stochastic reactor model (SRM)

The PDF–based Stochastic Reactor Model is derived from the joint composition PDF transport equation for scalars assuming statistical homogeneity and has been applied previously to HCCI/PCCI engine simulation [6, 20, 24]. The main feature of the SRM approach is that it can account for scalar micro-mixing and fluctuations in quantities unlike the multi-zone models. The same chemical mechanism as implemented in the CFD simulation was used. A Monte Carlo method with a second-order operator splitting technique was employed to solve the PDF transport equation. For the description of turbulent mixing, the Euclidean Minimal Spanning Tree (EMST) model [25] was used, in which particles undergoing mixing are chosen based on proximity in composition space. For further details, the authors recommend reference [20].

3.3 Sequential coupling of CFD and SRM

The direct integration of CFD and detailed chemical kinetics can take into account the influence of engine geometry on fuel and temperature distributions, however the computational cost is too high and uncertainties in the reaction rate closure influence model predictions. The PDF-based SRM with its detailed kinetics description has been demonstrated in our previous studies to successfully account for the inhomogeneities in temperature and composition and fluctuations at a low computational expense. The motivation of this work is to combine the intrinsic benefits of multi-dimensional CFD and the SRM approaches and develop a combined methodology for the modelling of PCCI combustion. The segregated sequential coupling methodology is essentially similar to the model proposed earlier [1]. In that, the 3D CFD simulation (without detailed kinetics description) was solved until a transition point, and then the results were mapped onto a combustion model. In our studies we found that the temperature-equivalence ratio $(T - \Phi)$ map resulting from the CFD calculation was sensitive to the inclusion of detailed kinetics within CFD.



(a) CFD (b) Downsampling

Figure 2: *T-Φ mapping between 3D CFD and SRM.*

Additionally, to account for the low temperature chemistry, the 3D CFD directly coupled with detailed chemical kinetics was solved from IVC until a transition point. The transition point was defined as the instant at which the maximum cell temperature just exceeds 960 K. At the transition point, the 3D information obtained from CFD was mapped into a 2D $(T-\Phi)$ space as shown in Figure 2(a). The $T-\Phi$ space was discretized into bins with intervals of 10 K and 0.02, respectively. In each 2D bin, the species mass fractions and temperature in the corresponding computational cells within the T- bands were averaged and passed back to the corresponding particles used for SRM as shown in Figure 2(b). It should be noted that all the liquid fuel left before the transition point was also mapped to the corresponding particles, in which the evaporation process was accounted for in the subsequent SRM simulation. Finally, the SRM simulation was started at the transition point and completed at EVO. Thus the methodology focuses on utilizing the detailed flow description capability of the KIVA code for taking into account the spray and combustion chamber geometry and then utilizes the SRM approach with detailed kinetics while approximating the flow description through the micro-mixing model parameter.

Table 2: *Comparison of measured and calculated emissions.*

	NO (ppm)	**CO (ppm)**	**uHC (ppm)**	**CO/CO$_2$**
Experiment	54.9	2673.0	190.0	0.21
Sim. with CFD-SRM	65.5	2722.0	376.0	0.32
Sim. with CFD	0.7	5225.0	2772.0	0.26

The models described above were used to simulate the Caterpillar 3406 MCTE. The nu-

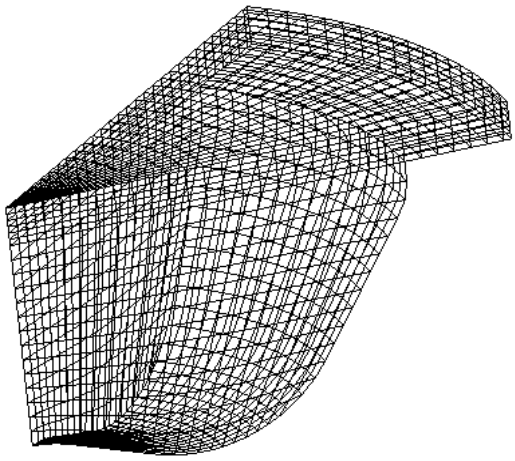


Figure 3: *Hexahedral mesh for the Caterpillar 3406 MCTE.*

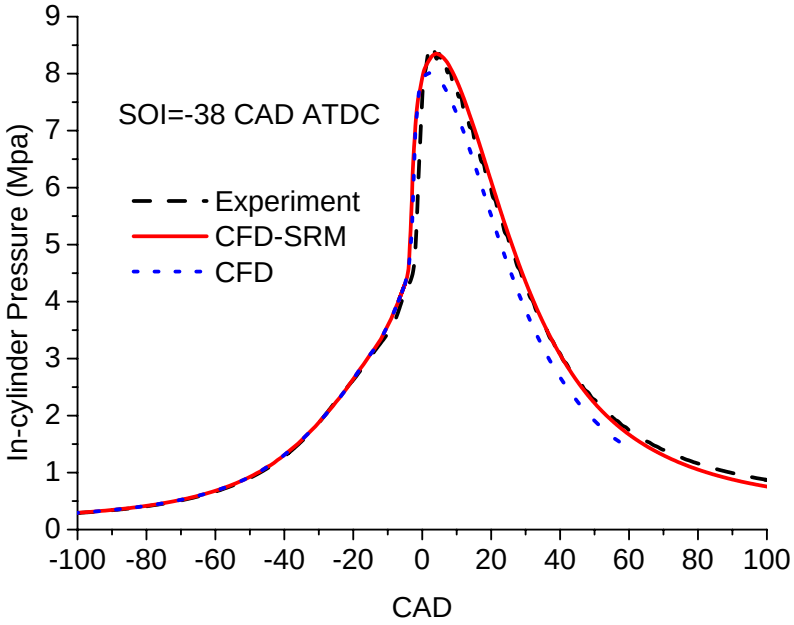


Figure 4: *Comparison of measured and calculated in-cylinder pressure.*

merical grid used for the analysis was a 3D 45 ° sector hexahedral grid with 30,000 cells at BDC as shown in Figure 3. The engine operating conditions for this study are listed in Table 1. The engine was operated at 1200 rpm. The fuel quantity of 0.147g was fixed for each injection. The start of injection was -38 ATDC and the spray included angle was 90 °. The direct coupling of CFD with full chemistry, together with the sequential coupling of CFD and SRM were chosen to simulate the selected validation case. In order to make a direct comparison between those two methods, the same n-heptane fuel chemistry mechanism, sub-models and model constants were used. The computational time for the sequential coupling of CFD and SRM is around 5 days (5 days for CFD with full chemistry running to the transition point 5 BTDC and 8 hours for using SRM to calculate the main combustion) using a desktop PC with 3.0 GHz CPU, as compared to 25 days CPU time using detailed solution with full chemistry in each cell. Note that 500 stochastic particles were used and the stochastic heat transfer parameter was set at 40 for the SRM approach, throughout the entire study. Figure 4 compares the measured and simulated pressure profiles. As shown in Figure 4, the pressure profile predicted by the sequential coupling of CFD and SRM matches with the experimental profile reasonably well. The predicted auto-ignition timing and pressure rise by using both methods are almost the same, although the direct coupling of CFD and chemistry under-predicts the peak and expansion pressure. This discrepancy will be explained later by referring to the detailed statistical plot comparisons. The predicted and measured pollutant emissions are compared in Table 2. The NO and CO emissions prediction correlates quite well with the measured ones, whereas the uHC are over-predicted by 50% as compared to the experiment. The over prediction in uHCs can be attributed to the uncertainties around the model parameters in the KH-RT spray model for such an early direct injection with fuel impinging on the cylinder wall.

Furthermore, the sequential CFD-SRM coupling was compared to the CFD coupled with detailed chemical kinetics on the basis of the evolution of the temperature - equivalence ratio $(T - \Phi)$ scatter. It should be noted that the notional particles governed by the PDF evolution in the SRM always correspond to certain fluid parcels in physical space. The $T - \Phi$ scatter plot of all notional particles (SRM) or computational cells (CFD) is shown in Figure 5. The statistical plot shows the combined effect of relatively hot temperature and near stoichiometric fuel-O2 equivalence ratio contribute to the earliest and fastest burn, while either rich or lean mixture leads to incomplete combustion, as indicated by the low combustion temperature as shown in Figure 5. There is a noticeable difference in thermal stratification between the statistics plots at a crank angle of 50 ATDC. This can be explained by the fact that the full chemistry based CFD approach does not consider the interaction of turbulence/chemistry. The turbulence mixing term in the SRM approach is closed using the EMST model, whereas the chemical source term appears in a closed form. The effect of turbulence/chemistry interaction increases the sub-grid homogeneity through micro-mixing, which was found to enhance the combustion and increase the peak pressure as compared to the CFD based model without considering turbulence/chemistry interactions [29]. This also explains higher uHC predicted by the full chemistry based

CFD model without considering turbulence/chemistry interactions, as compared with the measured quantities. However, the variance in composition predicted by both methods correlates reasonably well.

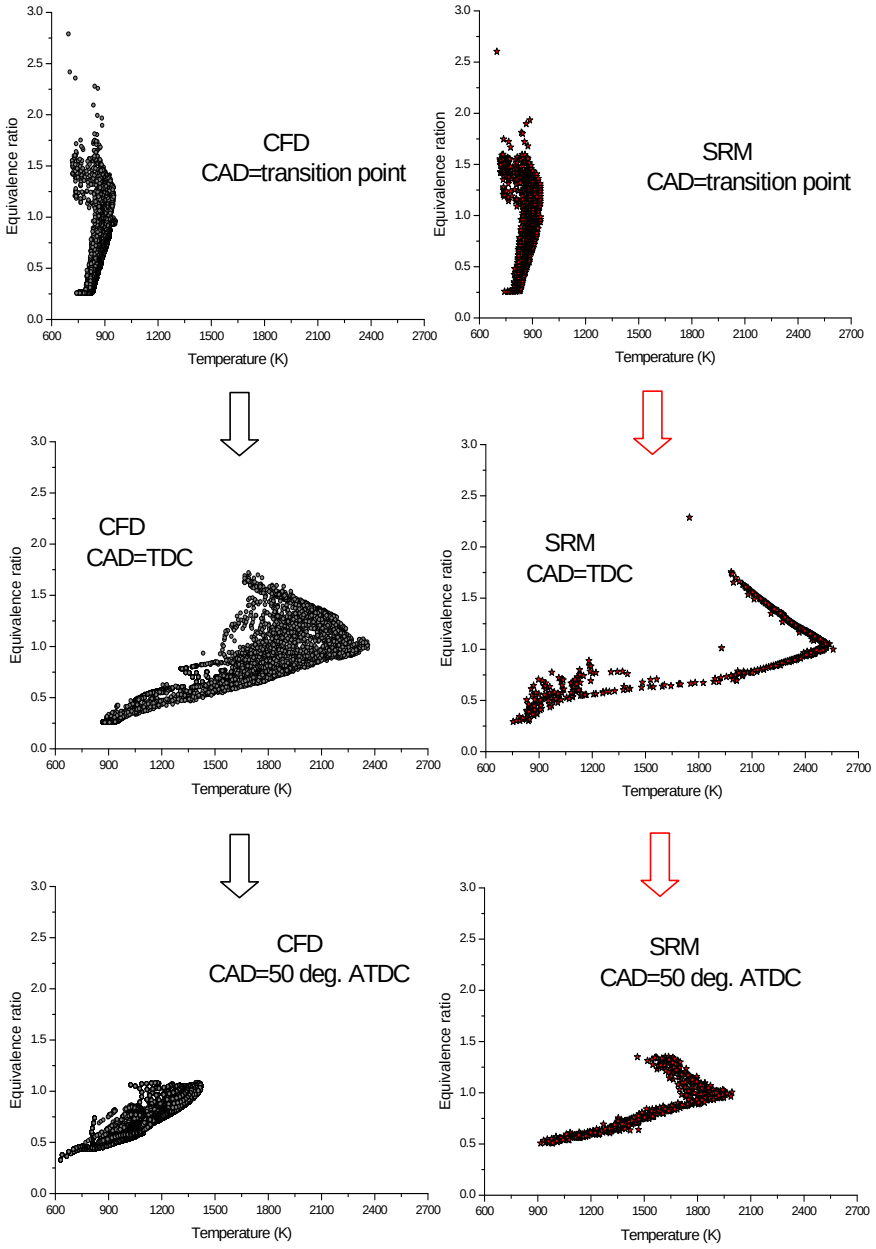


Figure 5: *T-Φ scatter cloud evolution for CFD and SRM after the transition point.*

4 Results and Discussion

4.1 Effect of injection timing sweep

In order to ensure sufficient time for mixing, the fuel injection in PCCI combustion mode is much more advanced as compared to that in conventional CIDI diesel engine. On account of the low volatility of diesel fuel, too early injection with the conventional wide spray angle injector in low ambient gas density could result in very serious spray impingement, wall wetting and reduced combustion efficiency leading to a corresponding rise in emissions [18]. Hence, to make a compromise between the residence time for mixing and wall wetting, the investigated injection timing sweep range was limited from -53 CAD to -38 CAD ATDC, and the injection duration was fixed as in Figure 1. The sequential 3D CFD - SRM approach was applied to carry out this parametric study related to the injection timing sweep. In our study, the empirical constant B_1 within the KH spray model that controls the secondary atomization rate was calibrated to 30 for the cases with relatively early injection i.e. at -53 CAD and -46 CAD ATDC, and equal to 20 for the cases with injection at -41 CAD and -38 CAD ATDC. All other model constants and initial conditions were kept same for all simulations. Figure 6 shows how the mixture quality varies with injection timing at the end of the compression stroke (-5 CAD ATDC). As shown in Figure 6, the mixture stratification increased as the injection was retarded. It can be observed that the earlier the ignition timing, the more homogeneous the mixture on account of the longer residence time for air-fuel mixing. The spatial equivalence ratio and temperature distributions between the two extreme injection cases (the most advanced and the most retarted injection cases) were compared, as depicted in Figure 7. It was observed that with the most advanced injection, the fuel rich mixtures were formed at the upper edge of the piston bowl with relatively low temperature, due to the charge cooling from fuel evaporation. This can also be seen as the upper left cells depicted in the scatter plot in Figure 7. It indicates that the charge cooling effect from fuel evaporation is dominant for mixtures leaner than stoichoimetric. In addition, the lean mixtures with relatively high temperature were found near the center and bottom of the piston bowl in the most advanced injection case. As compared to the case with injection at -53 CAD ATDC, more fuel rich mixtures $(\Phi > 1)$ can be seen at the edge of the piston bowl with relatively high temperature. This can be attributed to the richer fuel pockets in the retarded injection case which contribute towards higher low temperature heat release, as shown Figure 6 and Figure 7(b). Furthermore, the mixtures closer to the bowl wall in the range $0.8 < \Phi < 1.2$ experience an onset of cool flame chemistry and lead to increased stratification. Thus, these are the air-fuel mixtures responsible for reaching the temperature threshold of 960K. Figure 8 shows the comparison between the measured and the calculated in-cylinder pressure profiles as a function of injection timing. As compared to the experiment, a slightly earlier auto-ignition and lower peak pressure was predicted in the cases with injection at -46 CAD and -53 CAD ATDC.

However, in general the predicted pressure correlated reasonably well with the experimental one. The same pressure variation trends as a function of injection timing were seen between the simulation and the experiments. The ignition timing advanced with retarded injection timing as shown in Figure 8. This can be explained by the presence of fuel rich pockets described earlier (Figure 6).

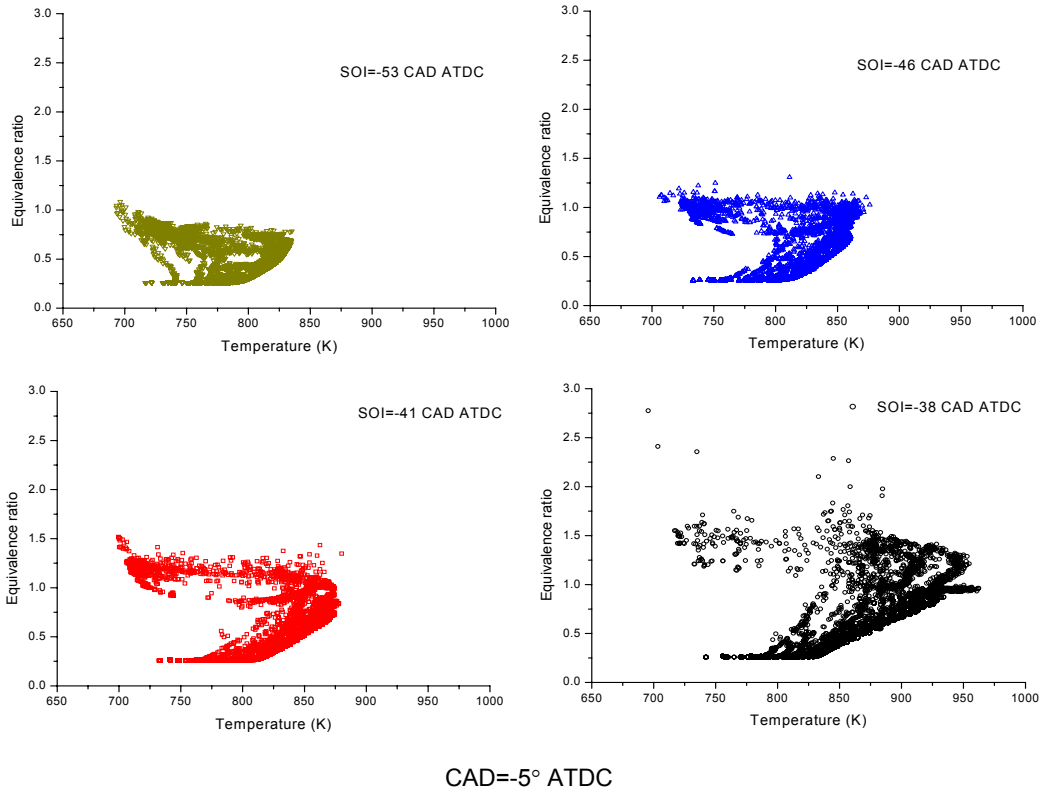
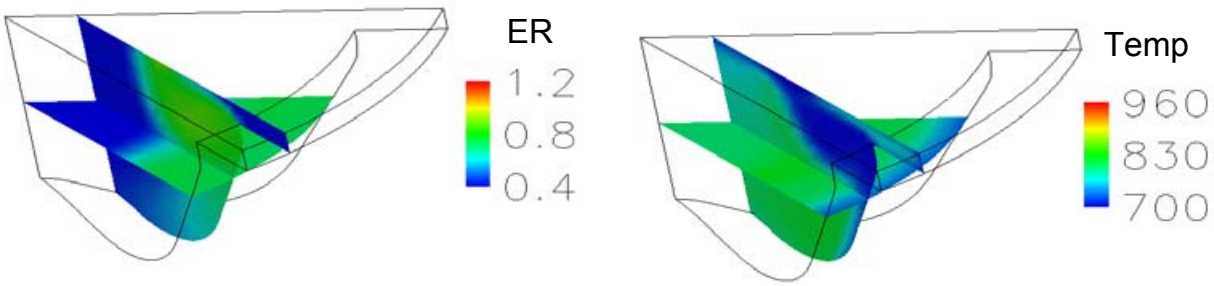


Figure 6: *T-ϕ statistical scatter plot at -5 CAD ATDC.*

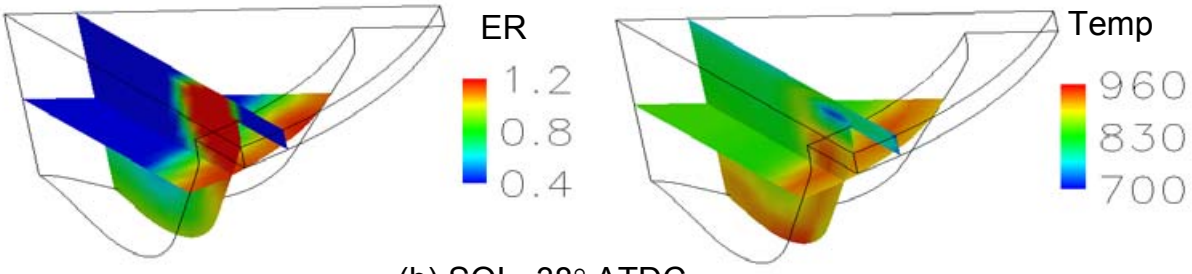
As indicated in Table 3, the predicted emissions match well with the measured ones, except a slight over-prediction of uHC. Figure 9 shows the CO and uHC emissions as a function of temperature and equivalence ratio at a crank angle of 50 CAD ATDC. Comparing the most advanced and the most retarded injection cases, higher CO was formed by the particles with slightly lean mixture and in the temperature range of 1300-1500 K in the most retarded injection case, which is consistent with a study published earlier [6]. In addition, higher uHC was found in the lean mixture with low temperature, due to the incomplete combustion in the advanced injection case.

Table 3: *Comparison of combustion parameters and emissions between the simulation and experiment for different injection timings.*

	SOI=-53°		SOI=-46°		SOI=-41°		SOI=-38°	
	Sim.	**Exp.**	**Sim.**	**Exp.**	**Sim.**	**Exp.**	**Sim.**	**Exp.**
10% MFB	6.1		0.7		-0.6		-3.65	
10-90% MFB	20.1		10.4		11.6		20.1	
$dP/dCAD_{max}$	0.7	0.6	1.5	1.0	2.0	1.5	1.9	1.7
P_{peak}(Mpa)	6.0	6.4	7.5	7.6	8.2	8.1	8.4	8.4
T_{peak}(K)	1460.0		1563.0		1639.0		1653.0	
NO (ppm)	34.0	77.0	64.9	68.9	59.4	63.7	65.5	54.9
CO (ppm)	2330.0	1747.0	2170.0	1626.0	1848.0	1750.0	2722.0	2673.0
uHC(ppm)	810.0	855.0	678.0	582.0	515.0	297.0	376.0	190.0



(a) SOI=-53° ATDC



(b) SOI=-38° ATDC

Figure 7: *Equivalence ratio (ER) and temperature distributions at -5 CAD ATDC.*

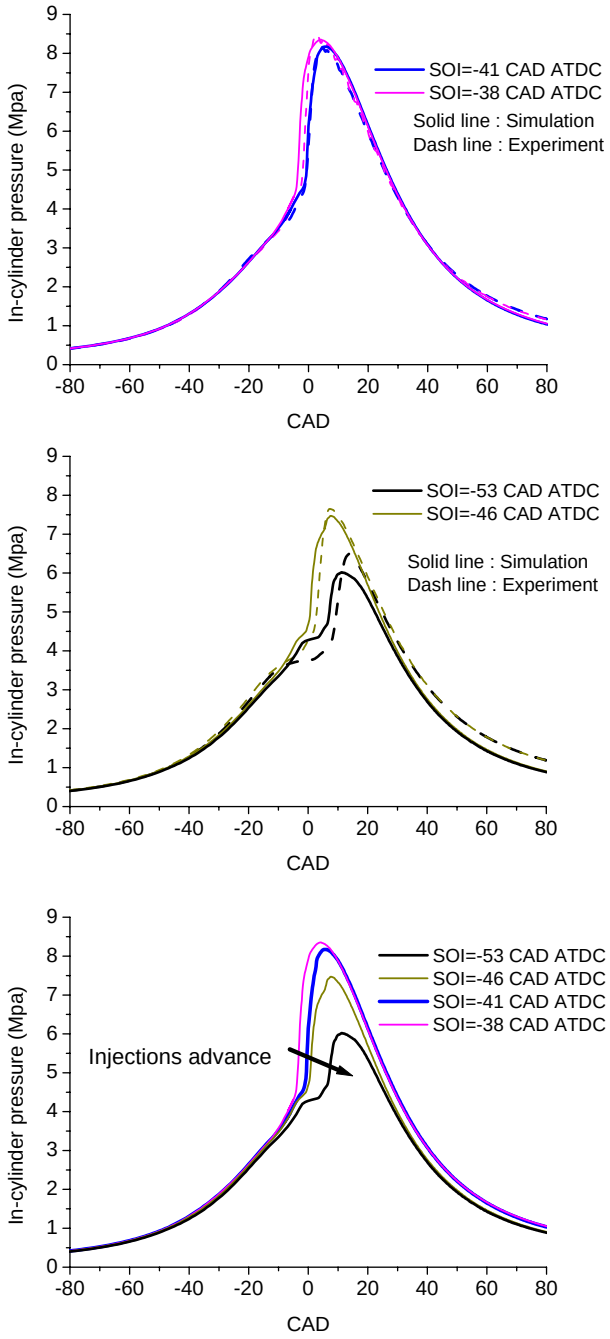
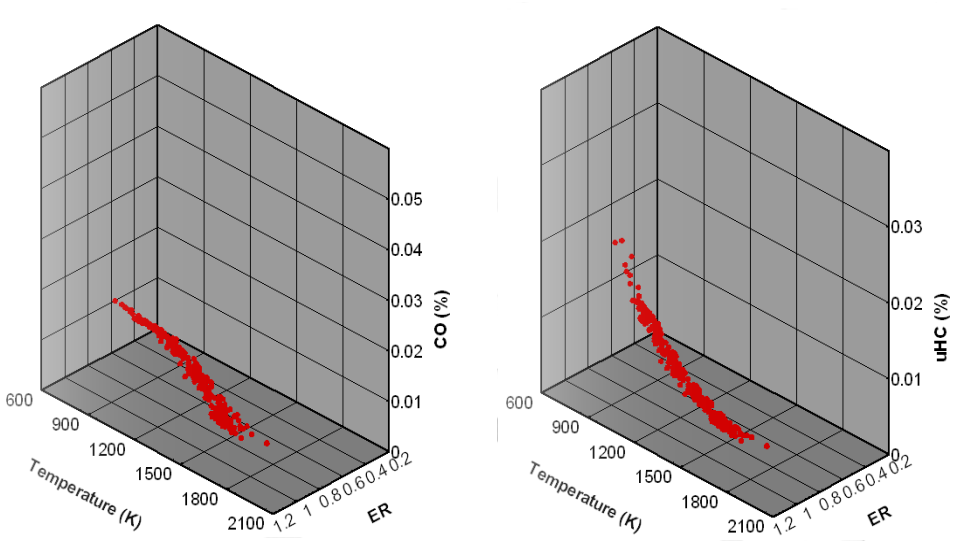
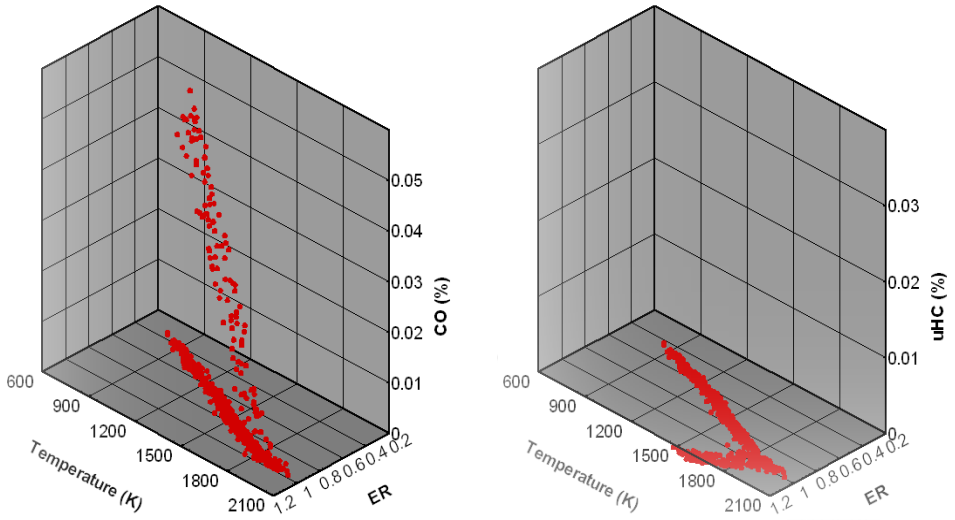


Figure 8: *Pressure profiles comparison between simulation and experiment for different injection timing cases.*



(a) SOI=-53° ATDC



(b) SOI=-38° ATDC

Figure 9: *Scatter plot of CO and uHC as a function of temperature and equivalence ratio at 50 CAD ATDC for the -53 and -38 CAD ATDC injection timings.*

4.2 Effect of bowl geometry

The role of piston geometry in generating turbulence and thereby reducing the rate of combustion (increasing the combustion duration in HCCI mode) has been investigated experimentally earlier [9, 27]. Recently, Shi et al. [23] employed genetic algorithms (GA) in conjunction with the KIVA code and proposed an optimal combination of spray targetting, bowl geometry and swirl ratio to reduce emissions and increase fuel efficiency in Diesel engines. Boyarski and Reitz [7] also applied GA-KIVA simulation tool to optimise the piston bowl geometry for early direct injection premixed compression ignition in a light duty Diesel engine. The modelling generated piston-bowl shape resulted in an open crater bowl as compared to the original re-entry bowl shaped piston. The development of sequential coupling methodology of 3D CFD and SRM is capable of capturing the engine geomoetry related information within the SRM approach. In this methodology, a direct coupling of CFD and full chemistry is responsible for the low temperature combustion and provides sufficient spatial information related to air-fuel mixing and chemical kinetics, whereas the SRM approach simulates the high temperature combustion part while accounting for turbulent micro-mixing, heat transfer and detailed chemistry. A parametric sensitivity study on the effect of bowl geometry on PCCI combustion and emissions was carried out using the integrated 3D CFD-SRM model. Figure 10 shows the three different engine bowl gemoetries investigated, namely open bowl, vertical side wall bowl and re-entry bowl. It should be noted that all the bowl cavity volume and bowl depth were kept same, aiming at retaining the same compression ratio (10:1). The same model constants and initial conditions were applied in all simulations with injection timing fixed at -38 CAD ATDC. Figure 11 and Figure 7(b) compare the equivalence ratio and temperature distributions for the three bowl shapes at a fixed crank angle of -5 CAD ATDC. It was observed that less fuel was distributed to the centre of the piston bowl in the case of the re-entry bowl shape, as compared to the other two bowl shapes, due to smaller impingement angle. Furthermore, most of the liquid fuel in the case of the re-entry bowl shape evaporated before the transition point (-5 CAD ATDC). In comparison with the other two piston configurations, the fuel close to the upper edge of the re-entry piston bowl evaporated relatively later as reflected by the low temperature pocket, on account of the evaporative cooling effect. In order to assess the mixture quality, the evolution of the T- statistical scatter for the three bowl shapes is shown in Figure 12. It should be noted that the overall mixture equivalence ratios for all three different bowl configurations were around 0.6. As shown in Figure 12, a more homogeneous lean mixture was observed in the re-entry bowl shape at -10 CAD ATDC, as compared to the other two bowl shapes. This indicates that the relatively strong squish flow in the re-entry bowl leads to faster fuel mixing near TDC. Figure 13 quantitatively assesses the mixture homogeneity according to the percentage of mixture in different equivalence ratio ranges $(\Phi > 1.2, 0.8 < \Phi < 1.2 and \Phi < 0.8)$.

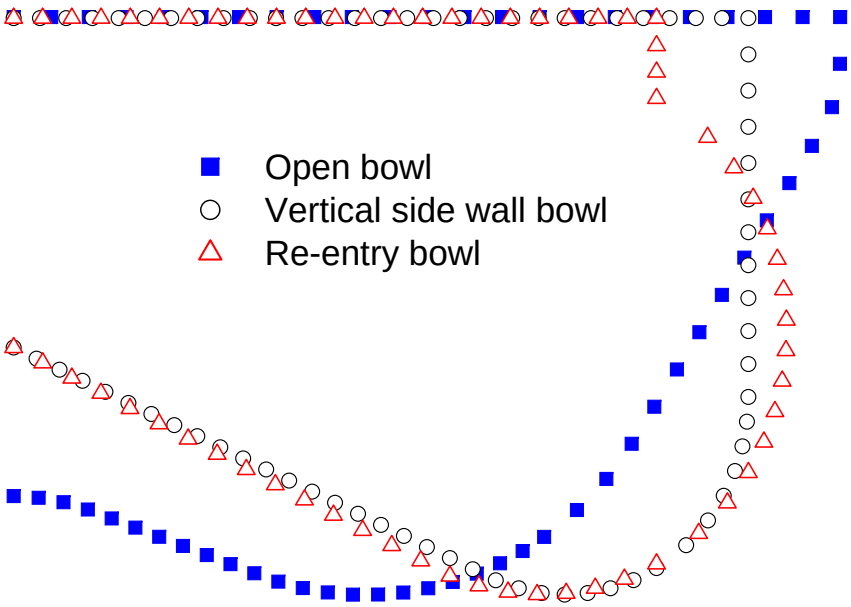


Figure 10: *Three engine bowl configurations (open, vertical side and re-entry type).*

As shown in Fig. 13, at the end of the compression stroke, 84% of the total charge in the re-entry bowl case was in the lean range, as compared to about 80% for the vertical wall bowl, and 76% for the open bowl shape. It was further confirmed that the re-entry bowl produced the most homogeneous mixture, whereas the most stratified mixture resulted in the case of the open bowl shape with 16% of the charge within the equivalence ratio range 0.8 to 1.2. Some degrees of stratification could be desirable in order to trigger the ignition. This is consistent with the observation in Figure 14, in which earlier ignition was seen in the open bowl shape on account of the presence of more relatively fuel rich pockets, when compared to the other two bowl shapes. Table 4 shows the predicted emissions for the three bowl shapes. Comparing the three bowl shapes, the highest CO emission was seen with the open bowl shape, while the highest uHC and the lowest NO emissions were observed in case of the re-entry bowl. The vertical side wall bowl shape produced the lowest combined CO and uHC emissions.

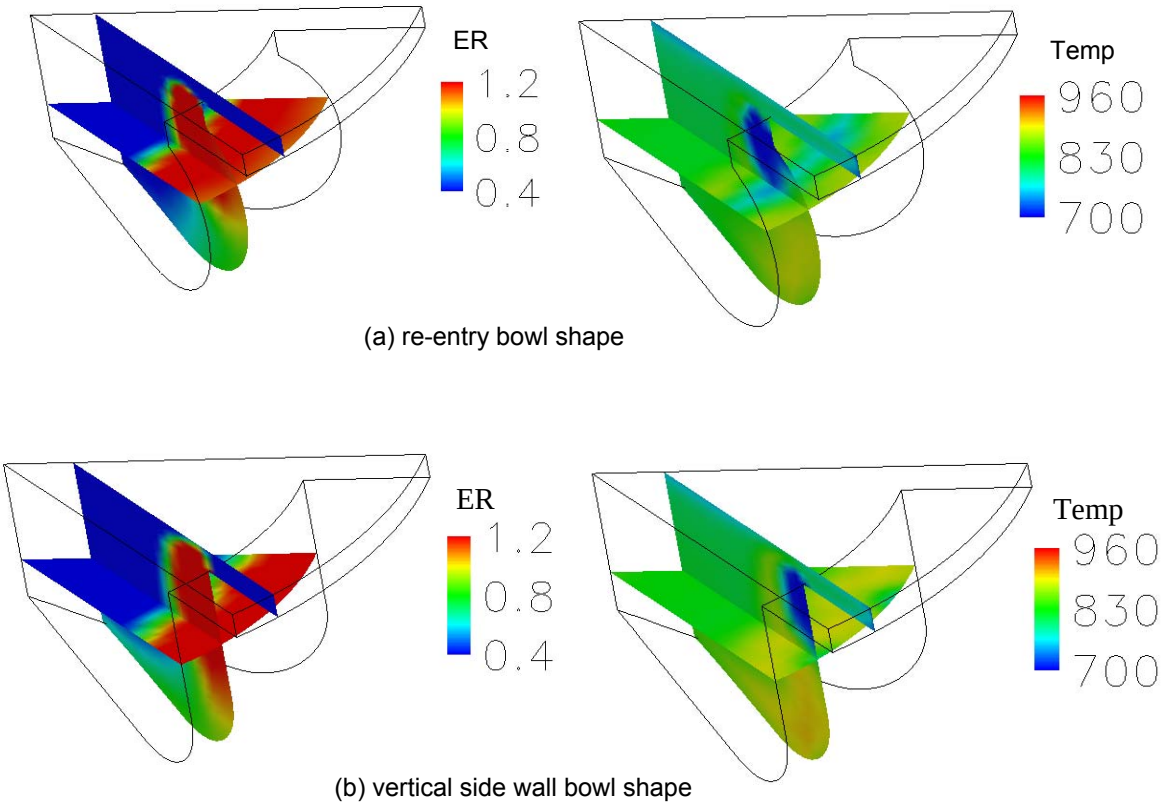


Figure 11: *Equivalence ratio and temperature distribution for re-entry and vertical bowls at crank angle of -5 CAD ATDC.*

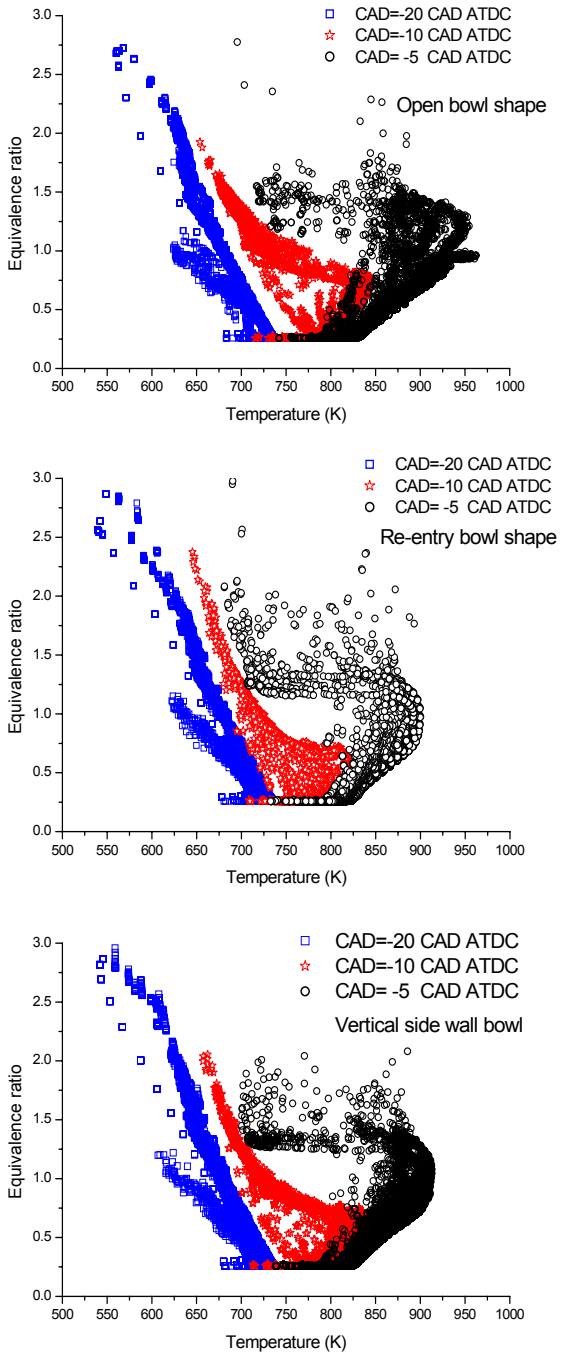
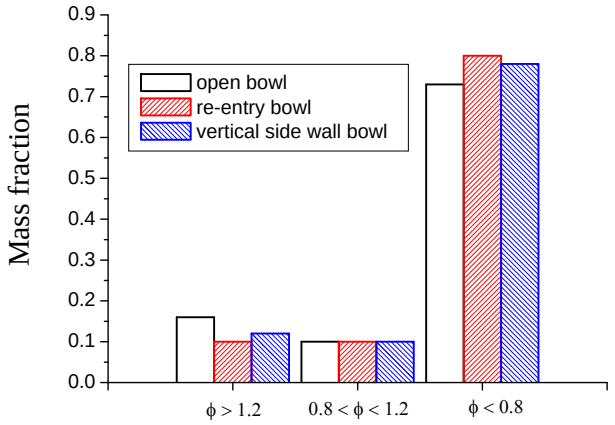


Figure 12: *T-ϕ statistics scatter plots for the three bowl shapes.*

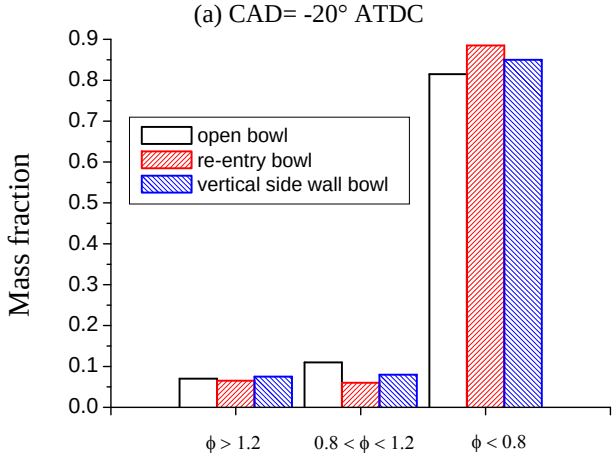
Overall, the integrated 3D CFD-SRM approach has been developed in order to reduce the computational expense in optimising the combustion chamber geometry. Further work in terms of experimental validation of the CFD-SRM calculations for a variety of piston geometries is important and will be the subject of future publications.

Table 4: *Emission comparison for the three bowl shapes.*

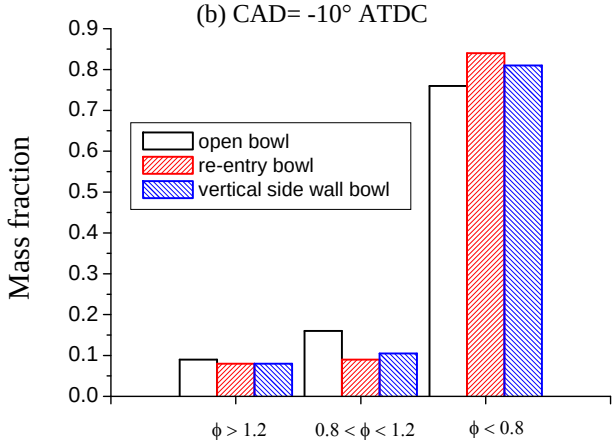
	NO (ppm)	**CO (ppm)**	**uHC (ppm)**
Open bowl	65.5	2722.0	376.0
Re-entry bowl	5.8	2480.0	580.0
Vertical side wall bowl	34.7	2450.0	482.0



(a) CAD= -20° ATDC



(b) CAD= -10° ATDC



(c) CAD= -5° ATDC

Figure 13: *Mass percentage of the charge within the equivalence ratio ranges for the three bowl shapes.*

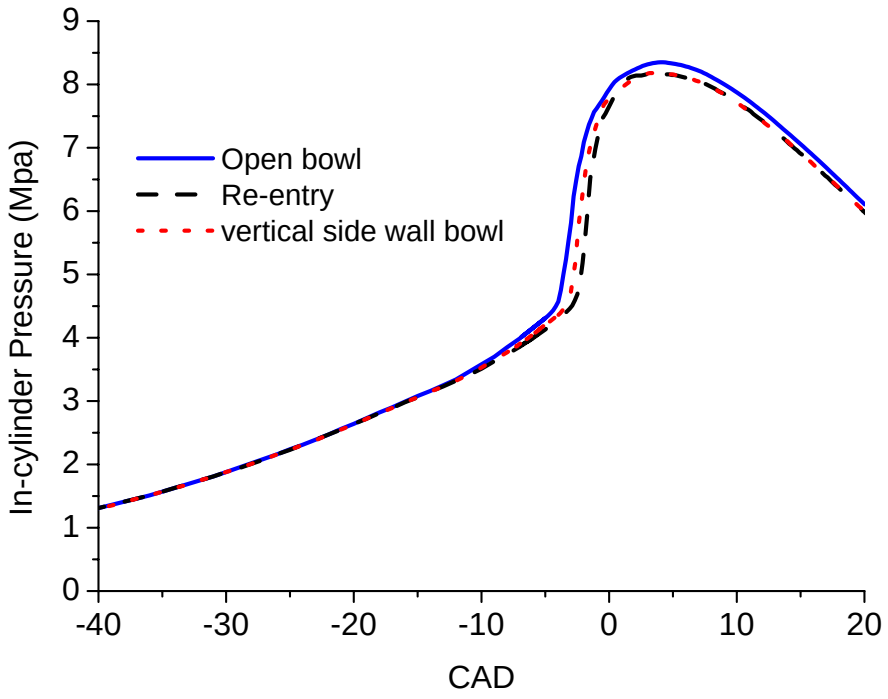


Figure 14: *Pressure profiles for the three bowl shapes.*

5 Conclusion

A sequential coupling methodology of 3D CFD and SRM was developed and applied to study the effects of injection timing sweeps and piston bowl geometries on PCCI combustion and emissions. In this approach, a CFD model with direct integration of detailed chemistry was adopted to provide sufficient chemical kinetics and engine geometry related information during the low temperature combustion, the SRM simulates the high temperature combustion, while accounting for turbulent micro-mixing, stochastic heat transfer and detailed chemical kinetics.

The integrated CFD-SRM model was validated against the measurements for a base case, and further compared with the direct coupling of CFD with the same detailed chemical description. A reasonably good agreement was achieved between both the modelling approaches and the experimental results for the in-cylinder pressure. However, the prediction of CO, uHC and NO emissions was improved with the CFD-SRM methodology.

Furthermore, the computational expense incurred by the CFD-SRM model was observed to be 75% lower than that with the direct coupling of CFD and kinetics.

The influence of injection timing on the air-fuel mixture preparation and consequently on the combustion and emissions was investigated using the coupled CFD-SRM methodology. The degree of mixture homogeneity as a function of injection timing was explained in terms of temperature-equivalence ratio $(T - \Phi)$ scatter. The most retarded injection timing resulted in locally rich air/fuel pockets $(1 \leq \Phi < 2,725 \leq T \leq 950)$ thereby triggering the low temperature chemistry and advancing the combustion phasing.

The integrated CFD-SRM approach can account for piston configuration and other combustion chamber geometry related information. The model was applied to investigate the effect of three bowl configurations (open, vertical wall and re-entry bowl shapes) on combustion and emissions. Comparing the three bowl shapes, the earliest combustion phasing, and highest NO and CO emissions were noted with the open bowl piston shape, whereas the lowest total CO and uHC emissions were observed in the case of the vertical side wall bowl.

6 Acknowledgments

This work has been partly funded by the Technology Strategy Board (TSB) and One NorthEast, UK, under the Validation of Complex Systems (VoCS) grant programme. Financial support has also been provided by the EPSRC (Engineering and Physical Sciences Research Council), UK, grant number EP/D068703/1.

References

[1] S. Aceves and D. L. Flowers. A Multi-zone Model for Prediction of HCCI Combustion and Emissions. SAE Paper 2000-01-0372, 2000.

[2] A. Amsden. KIVA–3V: A Blocked-structured KIVA Program for Engine with Vertical or Canted Valves. LA-13313-MS, 1997.

[3] A. Babajimopoulos, G. Lavoie, and D. N. Assanis. Modelling HCCI Combustion with High Levels of Residual Gas Fraction-A Comparison of two VVA Strategies. SAE paper 2003-01-3220, 2003.

[4] A. Babajimopoulos, D. N. Assanis, D. Flowers, and R. Hessel. A Fully Coupled Computational Fluid Dynamics and Multi-zone Model with Detailed Chemical Kinetics for the Simulation of Premixed Charge Compression Ignition Engines. *International Journal of Engine Research*, 6:497–512, 2005.

[5] A. Bhave, M. Kraft, L. Montorsi, and F. Mauss. Modelling a Dual Fuelled Multicylinder HCCI Engine Using a PDF based Engine Cycle Simulator. SAE paper 2007-01-0561, 2004.

[6] A. Bhave, M. Kraft, L. Montorsi, and F. Mauss. Sources of CO Emissions in an HCCI Engine: a Numerical Analysis. *Combustion and Flame*, 114:634–637, 2006.

[7] N. J. Boyarski and R. D. Reitz. Premixed Compression Ignition (PCI) Combustion with Modeling Generated Bowl Geometry, in a Diesel Engine. SAE paper 2006-01-0198, 2006.

[8] L. Cao, H. Su, S. Mosbach, A. Bhave, M. Kraft, S. Kook, and C. Bae. Studying of the Influence of Direct Injection on PCCI Combustion and Emissions at Engine Idle Condition Using Two dimensional CFD and Stochastic Reactor Model. SAE paper 2008-01-0021, 2008.

[9] M. Christensen, B. Johansson, and A. Hultqvist. The Effect of Combustion Chamber Geometry on HCCI Operation. SAE paper 2002-01-0425, 2002.

[10] D. J. Cook, H. Pitsch, J. H. Chen, and E. Hawkes. Flamelet based Modeling of Autoignition with Thermal Inhomogeneities for Application to HCCI Engines. *Proceedings of the Combustion Institute*, 31:2903–2911, 2007.

[11] D. Flowers, S. Aceves, R. Martinez, R. Hessel, and R. W. Dibble. Effect of Mixing on Hydrocarbon and Carbon Monoxide Emissions Prediction for Isooctane HCCI Engine Combustion using A Multi-zone Detailed Kinetics Solver. SAE paper 2003-01-1821, 2003.

[12] E. Hairer and G. Wanner. Solving Ordinary Differential Equations II - Stiff and Differential Algebraic Problems. Springer-Verlag, 1991.

[13] Z. Han and R. Reitz. A Temperature Wall Function Formulation for Variable-Density Turbulent Flows with Application to Engine Convective Heat Transfer Modelling. *International Journal of Heat and Mass Transfer*, 40:40–60, 1997.

[14] R. Jhavar and C. Rutland. Effects of Mixing of Early Injection Diesel Combustion. SAE paper 2005-01-0154, 2005.

[15] S. Kong and R. Reitz. Application of Detailed Chemistry and CFD for Predicting Direct Injection HCCI Engine Combustion and Emissions. *Proceedings of the Combustion Institute*, 29:667–669, 2002.

[16] S. Kong, N. Ayoub, and R. Reitz. Modeling Combustion in Compression Ignition Homogeneous Charge Engines. SAE paper 920512, 1992.

[17] S. C. Kong, C. Marriot, R. Reitz, and M. Christensen. Modeling and Experiments of HCCI Combustion Using Detailed Chemical Kinetics with Multi-dimensional CFD. SAE paper 2001-01-1026, 2001.

[18] S. C. Kong, H. Kim, R. D. Reitz, and Y. Kim. Comparisons of Combustion Simulation Using Representative Interactive Flamelet Model and Direct Integration of CFD with Detailed Chemistry. *ASME Journal of Gas Turbines and Power*, 129:252–260, 2007.

[19] H. Lehtiniemi, Y. Zhang, R. Rawat, and F. Mauss. Efficient 3D CFD Combustion Modeling with Transient Flamelet Models. SAE paper 2008-01-0957, 2008.

[20] S. Mosbach, H. Su, M. Kraft, A. Bhave, Z. Wang, and J. Wang. Dual Injection HCCI Engine Simulation using a Stochastic Reactor Model. *International Journal of Engine Research*, 8:41–50, 2007.

[21] P. O'Rourke and A. A. Amsden. A Spray/Wall Interaction Submodel for the KIVA-3 Wall Film Model. SAE paper 2000-01-0271, 2000.

[22] M. A. Patterson and R. D. Reitz. Modelling the Effect of Fuel Spray Characteristics on Diesel Engine Combustion and Emissions. SAE Paper 980131, 1998.

[23] Y. Shi and R. D. Reitz. Optimization Methodologies to Study the Effects of Bowl Geometry, Spray Targeting and Swirl Ratio for a Heavy-Duty Diesel Engine Operated at High Load. SAE paper 2008-01-0949, 2008.

[24] H. Su, S. Mosbach, M. Kraft, A. Bhave, S. Kook, and C. Bae. Two-stage Fuel Direct Injection in a Diesel Fuelled HCCI Engine. SAE paper 2007-01-1880, 2007.

[25] S. Subramaniam and S. B. Pope. A Mixing Model for Turbulent Reactive Flows based on Euclidean minimum Spanning Trees. *Combustion and Flame*, 115:487–514, 1998.

[26] M. Tunér, M. Pasternak, H. Bensler, and F. Mauss. A PDF based Model for Full Cycle Simulation of Direct Injected Engines. SAE paper 2008-01-1606, 2008.

[27] A. Vressner, A. Hultqvist, and B. Johansson. Study on Combustion Chamber Geometry effects in an HCCI Engine Using High-Speed Cycle-Resolved Chemiluminescence Imaging. SAE paper 2007-01-0217, 2007.

[28] Y. Yu, W. H. Su, and H. Z. Huang. Study of Fuel Distribution on Diesel PCCI Combustion by Development of a New Characteristic-time Combustion Model. SAE paper 2008-01-1605, 2008.

[29] Y. Z. Zhang, E. Kung, and D. Haworth. A PDF Method for Multi-dimensional Modelling of HCCI Engine Combustion: Effects of Turbulence/Chemistry Interactions on Ignition Timing and Emissions. *Proceedings of the Combustion Institute*, 30: 2763–2771, 2005.