Simulating PM emissions and combustion stability in gasoline/diesel fuelled engines

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Abstract

Regulations on emissions from diesel and gasoline fuelled engines are becoming more stringent in all parts of the world. Hence there is a great deal of interest in developing advanced combustion systems that offer the efficiency of a diesel engine, but with low PM and NO_x. One promising approach is that of Partially-Premixed Compression Ignition (PPCI) or Low Temperature Combustion (LTC). Using this approach, PM can be reduced in compression ignition engines by promoting the mixing of fuel and air prior to combustion.

This paper describes the application of an advanced combustion simulator for fuels, combustion and emissions to analyze the key processes which occur in PPCI combustion mode. A detailed chemical kinetic model with advanced PM population balance sub-model is employed in a PPCI engine context to examine the impact of ignition resistance on combustion, mixing, ignition and emissions. The ignition and combustion of a diesel-like fuel (n-heptane) and low octane gasoline-like fuel (84PRF) are compared using the model highlighting how the diesel-like fuel ignites at very rich equivalence ratios whereas the gasoline-like fuel ignites on the lean side. Sources of exhaust gas emissions are also identified.

For the first time, a computational model is employed to demonstrate the tradeoff between low PM emissions and "over-mixing" (sensitivity to cycle-to-cycle variations and combustion instability) for a full range of fuels with increasing ignition resistance. These results are then discussed noting that conventional hydrocarbon fuels which fulfill either a conventional diesel or gasoline standards are not necessarily consistent with those required to run an engine operating at it's optimal point in terms of PM emissions and combustion stability.

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1 Introduction

Driven by increasing regulation, the efficiency of gasoline and diesel engines and their associated exhaust gas emissions have improved dramatically over the last 25 years [29]. A major contribution has come through the adoption of virtual engineering tools which reduce development timescales and cost through offering engineers physical insight into complex interacting processes, facilitate design of experiments, engineering optimization, and most importantly enabling highly specialized expertise and analysis to be adopted by its users.

Virtual engineering tools applicable to in-cylinder combustion can be separated into three groups, (a) 0/1D cycle multi-cycle simulation tools (solving in less than a second per engine cycle) which are used widely for IC engine development for IMEP, engine breathing turbocharger matching etc. [1] however these codes generally adopt simple combustion models and take no account of in-cylinder stratification; (b) 3D CFD codes (solving in hours, days or weeks) which properly account for in-cylinder stratification and are employed for analysis of heat transfer, mixture preparation (spray distributions) however due to high associated computational cost in order to be used effectively these often employ heavily reduced, empirical "rules-of-thumb" to account for the chemistry of combustion, or succumb to the lack of robust turbulent reaction closure measures [24, 28], and (c) stochastic reactor codes [10, 17] (solving in seconds, minute or hours) which transform the in-cylinder geometry into a multi-dimensional Probability Density Function (PDF) of in-cylinder composition.

The implementation of detailed chemistry into IC engine combustion models has been carried out by a number of research groups [12, 15, 16], however generally the scope of these kinds of study have been limited to adoption within the limitations of 3D CFD (computational time) or 0/1D (no accounting for emissions/in-cylinder stratification) solutions. Due to the need to map out potential combinations of varying engine technologies, a rapid solution containing sufficient physical insight and ability to account of exhaust gas emissions has solutions is required. In recent years, the Stochastic Reactor Models have received an increasing amount of attention from the academic and industrial community as they offer the ability to full cycle simulation, compute combustion characteristics and exhaust gas emissions in manageable timescales through direct coupling with 0/1D cycle codes [2, 7, 17].

Stochastic reactor models (SRM) enable characterization of in-cylinder stratification but at a reduced computational cost compared to say 3D CFD [6, 12, 15, 16, 28], thus enabling easy adoption of advanced fuel oxidation and emissions models in timescales suitable for adoption into standard multi-cycle simulations [2, 7, 8]. Fuel oxidation and emissions formation models have seen considerable development over the proceeding ten years. Systematic development has advanced through the hydrocarbons building on the chemistry of smaller molecules (i.e. methane [26]) up to those relevant to gasoline and diesel surrogates of varying complexity (n-heptane/iso-octane [18, 23]). These models describe the complex interaction between chemical species reaction-by-reaction enabling robust computations of critical combustion processes such as ignition, autoignition, extinction, flame propagation and emissions formation including PM, NO_x, uHCs and CO [3, 5– 8, 10, 13, 18–22, 25, 27]. In the past, this approach has also been applied to simulate engines operated on duel and multiple fuel types [3, 19, 20, 27], including advanced octane blending [18] for surrogates.

The results of applying the SRM to kinetically-controlled combustion processes such as Homogenous Charge Compression Ignition (HCCI) have been published previously [3, 5, 7, 18–22, 24, 27], and the model has proven highly effective in characterizing combustion characteristics as well as exhaust gas emissions. These models have recently been extended to diesel fuelled combustion [22, 25], thus enabling the simulation of mixing controlled combustion yielding results in terms of heat release and exhaust gas emissions.

This paper bridges the gap between Compression Ignition Direct Injection CIDI and HCCI by examining fuel effects on Partially-Premixed Compression Ignition (PPCI) by increasing the resistance of the fuel to ignition and observing the transition from mixing controlled combustion to kinetically-controlled combustion.

Experimental data obtained by Kalghatgi [13, 14] was employed to validate a stochastic reactor model named SRM SUITE using a detailed fuel model including NO_x and PM chemistry for primary reference fuels. The model was then employed to examine the history of each particle in terms of temperature and equivalence ratio, demonstrating that ignition occurred in the rich regions of the combustion chamber for n-heptane, whereas for the 84PRF, increased ignition resistance and turbulent mixing resulted in ignition in the leaner regions.

A parametric study was then completed to examine the impact of fuel ignition resistance and injection timing upon Combustion Delay (CD), NO_x and PM. This exercise demonstrates for the first time from a computational model that as ignition resistance increases, combustion delay increases thus tendency reducing in PM is observed. Conversely, this same study also demonstrated the impact of so called "over-mixing" which resulted in poor combustion stability and increased sensitivity to cycle-to-cycle variations for fuels with a greater resistance to ignition.

2 Experiments

The experiments were performed on a 4-valve single-cylinder research engine, a full description of the experiments can be found in Kalgahtgi et al. [13, 14]. The engine had a bowl-in-piston geometry, with dimensions as presented in Table 1. Fuel was injected in a single pulse via a Bosch 7 hole injector, with injector cone angle of 153 and hole diameters of 0.13 mm, fed by an independent fuel supply rig. In-cylinder pressure was measured with a water-cooled pressure transducer (Kistler 6041A).

After a stabilization period, the emissions were logged once per second for 120 seconds and the average of those 120 recordings are used in this paper. At the same time, the in-cylinder pressure was recorded for 250 cycles. The operating condition, without EGR, is set out in Table 2. For a given fuel, the fuel flow rate was adjusted until the target IMEP in Table 2 was reached. In addition, the start of injection (SOI) was varied. SOI is the crank angle at which the electrical pulse to open the injector is initiated.

The fuel properties are set out in Table 3. An 84PRF was adopted as a simple surrogate

Compression Ratio (-)	15.9:1
Displacement (litres)	0.537
Bore (mm)	88
Stroke (mm)	88.3
Connecting Rod Length (mm)	149
Inlet valve open (IVO)	362 CAD
Inlet valve close (IVC)	595 CAD
Exhaust valve open (EVO)	143 CAD
Exhaust valve close (EVC)	385 CAD

 Table 1: Engine specification.

 Table 2: Engine operating point.

Speed (RPM)	1200
Manifold pressure (bar) (a)	1.0
Manifold temperature (deg C)	65
Exhaust pressure (bar) (a)	1.0
IMEP (bar)	4.0
Injection pressure (bar)	650
Equivalence ratio	0.370
Air mass flow rate (g/s)	6.03

for commercial gasoline, with an octane rating of 84, it might be considered not as resistant as commercial gasolines with a RON of greater than 95, however lower octane rated gasolines are considered more appropriate for PPCI applications [13]. As a surrogate for commercial diesel, n-heptane was adopted for this study. Whilst more advanced surrogates for both gasoline and diesel could have been employed for this study [18, 23], the adoption of iso-octane/n-heptane blends has a number of advantages. These blends are (a) well characterized in terms of chemical kinetic reaction rates and fundamental understanding/data, (b) in examining simple trends expressed later in the paper - a bicomponent blending model reduces the complexity of the analysis. An increase in the complexity of the surrogate employed (tri-, quad- or more components) as representative of practical gasoline/diesel fuels is a suitable topic for future investigations.

	84 PRF	n-heptane
RON	84	0
MON	84	0
vol. % of iso-octane	84	0
vol. % of n-heptane	16	100
Density (g/cc)	0.682	0.632
С	7.83	7.0
Н	17.67	16.0
LHV (MJ/Kg)	44.4	44.6

Table 3: Fuel properties.

3 Model

The SRM SUITE is an advanced combustion simulation tool which was derived from the Stochastic Reactor Model (SRM) that has been used in many previous studies [3, 5, 18– 22, 25, 27]. It is employed to simulate in-cylinder processes such as compression, heat transfer, mixture preparation, combustion, pollutant formation and expansion from inlet valve closure (IVC) to exhaust valve opening (EVO). These processes are simulated by considering both global and local quantities within the in-cylinder compositional space. Global quantities are total mass, volume, mean density and pressure; these do not vary within the combustion chamber. However local quantities such as chemical species mass fractions (i.e. fuel, oxidant, nitrogen, active species, pollutants, exhaust gases etc.) and temperature are assumed to be stratified within the in-cylinder compositional space. Both global and local quantities are allowed to evolve with respect to time by allowing these scalars to be influenced by the process of changing the cylinder volume with respect to crank angle and solving chemical kinetic reaction schemes. In addition, advanced submodels which simulate heat transfer, turbulent mixing and fuel injection have been applied. These are generally applied by allowing individual stochastic particles (selected on the basis of having similar composition) to interact by exchanging gas composition (fuel, chemical species etc.) as well as heat (or heat to the wall), the frequency of these interactions is controlled by the turbulent mixing timescale. The initial in-cylinder composition air and EGR is assumed homogeneous in terms of temperature, as the computation continues over time stratification increases. As would be expected, once a fuel injection event occurs, fuel stratification is the main source of inhomogeneity in terms of heat release and emissions formation.

By translating the in-cylinder compositional state from 3D space, as in the case of 3D CFD which requires thousands of grid points, to a PDF comprised of one hundred stochastic particles significant gains of computational cost are obtained. Previous studies have demonstrated computational times can be shortened by factors of 6000 (i.e. from months to minutes) without significant loss in model robustness [6, 7] enabling its adoption into industry standard multi-cycle 1D engine simulation tools.

This study extends the application of the simulator to PPCI combustion. The model was set-up according to the information in Table 4. Whilst no EGR was reported in the experiments, it was anticipated that around 5% of the charge would be internally trapped exhaust gas residuals. The default fuel oxidation and emissions formation model was employed which contained 872 reactions and 188 chemical species including a detailed description of NO_x and PM chemistry.

Given the increasing regulation in terms of size, number and morphology of PM produced by IC engines. a soot population balance sub-model has been developed and is employed in this study, a full description of its implementation is presented in more detail in [9, 13, 14, 22, 25], however a brief summary is as follows. A detailed set of population balance equations is used to model PM formation. The surface area, number of primary particles, primary particle diameters, of each aggregate are tracked including the number of carbon atoms, hydrogen atoms, PAH moles as well as the number of functional sites. Surface chemistry is also considered including the oxidation reactions.

Computation of a single cycle was completed in 6 minutes on a 12 processor machine [7].

Internal EGR (mass fraction)	0.05
Stochastic heat transfer Constant	2000
Turbulent mixing time (ms)	1.2
Turbulent mixing model	EMST
Injection model	PDF Based
Fuel model	PRF cmcl v1.2 detailed mechanism with PM and NO_x chemistry
Computational time (single processor)(Minutes)	60
Computational time (twelve processors)(Minutes)	6

Tabl	le 4:	Mod	el in	puts
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The model was parameterized by fixing the stochastic heat transfer constant to 2000 and the number of stochastic particles to 100, both these parameters have proven to result in a well resolved solution for heat release and emissions over a wide range of applications [3, 5, 18–22, 25, 27]. The model was resolved 500 times over feasible ranges of the "unknown" model inputs and model parameters, these were the turbulent mixing time and injection spray distribution. The best set were identified by comparing model and experiment for peak pressure, 50% MFB timing, combustion duration and NO_x emissions. Once identified, model parameters were fixed throughout the study.

4 Comparison of experimental and model results

4.1 (A) Comparison of pressure profiles

The resulting simulations for the n-heptane and 84PRF are presented in Figure 1. These are for the same SOI=-8.0 CAD aTDC. As observed experimentally the heat release is rapid at around TDC for n-heptane and at around 5CAD aTDC for the 84PRF, both the model and experiment agree well. Ignition for the 84PRF takes longer due to an increased concentration of iso-octane, it is more resistant to ignition, this observation is consistent with the reported octane numbers of the fuels as well as reported ignition delay times [11].



Figure 1: In-cylinder pressure vs. crank angle.

4.2 (B) Injection sweep

Next the timing of injection was varied as a blind test of the model, results are presented in Figure 2a. Presented in the diagram are the timing of 50% of Mass Fraction Burned (MFB) compared with the Combustion Delay (CD). As 50% MFB was delayed the CD is extended due to a lower in-cylinder temperature at the point of injection. Whilst the methods for obtaining the 50% MFB and CD between experiment (from the AVL data processing software) and the model outlined above were not identical, the resulting model results also satisfactorily mimic these same trends.

Peak pressures presented in Figure 2b are slightly lower than reported in the experiments, For later ignition times, the peak pressure associated with that due to compression alone (i.e. at TDC) proved to be the highest peak pressure noted in the models and experiments.

When compared in terms of exhaust gas emissions, in this case in terms of NO_x in Figure 2c, the trends and absolute values are mimicked well for the 84PRF, whereas those for the n-heptane fuelling are around 500ppm too high - this will be discussed in more detail in a later section.

Emissions of uHCs and CO are presented in Figure 2d and Figure 2e respectively. Absolute values and trends of uHCs and CO are reproduced well by the model for n-heptane, whereas those for the 84PRF the uHCs do not predict the step change in uHCs and steady increase in CO for later injection timings. These are simulations of mean pressure profiles, whereas the reported emissions are averaged over a number of successive cycles, and as noted in a later section, higher octane rated fuels are more sensitive to cycle-to-cycle variations and likely to produce partial combustion products, thus this is possible source of these differences.

Finally in Figure 2f, the emissions of PM are presented for both the model and experiment. The concentration of soot produced experimentally was small relative the uncertainty associated with the observation hence uncertainty bounds have been added. No PM was reported for the 84PRF whereas for earlier 50% MFB times, PM was observed experimentally for the n-heptane fuel. Consistent with studies of PM formation in DISI [9] and HCCI engines [22], the trends observed experimentally are reproduced by the model.

5 Further insight into experimental observations

The in-cylinder composition is presented in Figure 3a in terms of local temperature and equivalence ratio at -4.0, -2.0, -1.4, 0, 2.0 and 4.0 CAD aTDC for both the n-heptane and 84PRF blends with an injection timing of -8.0 CAD aTDC. At -4.0 and -2.0, the distribution of particles (in-cylinder fuel-air parcels) is linear, i.e. as injection has occurred, it has resulted in rich and lean particles- with richer particles at a lower temperature due to charge evaporation. At -2.0 CAD aTDC, the subtle difference on the rich side is associated with some low temperature (cool flame) heat release from the n-heptane flame. This results in thermal runaway in the richest particles and combustion continues from rich to lean particles in the n-heptane case, this is observed at -1.4 CAD aTDC and at TDC. Also presented in these same diagrams are the regimes of excessive PM and NO_x formation. As observed at -1.4 CAD aTDC, some of the stochastic particles move through the regime of high PM formation, in Figure 4 the computed PM size distribution is presented for a range of CAD timings. As the combustion event continues, the richest regions become leaner as they mix with unburned air. This increases the rate of re-oxidization reactions on the surface of the PM begins, thus reducing the total number of soot particles over time.

Ignition of the 84PRF is much later in the cycle, allowing more time for turbulent mixing, and ignition occurs at around an equivalence ratio of 0.6. Ignition then occurs in both the lean and rich directions, however the overall mixture was burned at a more homogeneous mixture distribution and avoided those regimes associated with excessive PM formation.

The rate of pressure rise for the model (as presented in Figure 1) proved slower than reported in the experiments, in addition the concentration of NO_x proved too high by 500ppm for the n-heptane case - as observed in the in-cylinder distributions above this



Figure 2: Injection timing sweep



Figure 3: In-cylinder local equivalence ratio versus temperature



Figure 4: Computed in-cylinder PM size distributions with respect to CAD for the nheptane fuelled case

could have been associated with either or a combination of (i) the distribution of air-fuel particles being too great thus the distribution of ignition delay times are greater resulting in slower combustion rates, (ii) an inadequate fuel oxidation model, or (iii) poor model parameterization. However when compared generally across the experimental the performance of the model is very good in terms of heat release and emissions, hence whilst model performance improvements can be made (and development is on-going), the overall performance of the model was considered satisfactory for further adoption in parametric studies.

6 Parametric study - impact of the resistance to ignition

6.1 Combustion delay

To characterize the impact of fuel effects on combustion and emissions, a parametric exercise was carried out requiring a further 340 resolutions of the model. Ignition timing sweeps from -15.0 to 0 CAD aTDC in 0.5 CAD increments were carried out to determine the injection CAD for 50%MFB - presented in Figure 5 are the resulting data for a 50%MFB at 5CAD aTDC for increasing octane number or increasing resistance to ignition. Figure 5a shows that as octane number is increased the required SOI to achieve a 50%MFB at 5.0 CAD aTDC must be advanced. Similarly the observed Combustion Delay (CD) is also extended.

Presented in Figure 5b are the corresponding mixture compositions at the point of ignition.

The local equivalence ratio in the stochastic particle which ignited and burned first are presented as a function of octane number, as octane number is increased the corresponding equivalence ratio is reduced. Given the range of observed in-cylinder equivalence ratios presented in Figure 5b, and the observation that ignition occurs from an equivalence ratio of 2.5 to 0.4, this highlights the importance of the adoption of detailed chemical models over reduced chemical or "rule-of-thumb" solutions which are often simplified by limiting their application to smaller ranges of equivalence ratio, for example the rich chemistry is often neglected in HCCI applications [4].

6.2 Exhaust gas emissions

As octane number increases the PM is reduced. The reduction of PM for increasing octane rating is consistent with the experimental observations of Kalghatgi et al. [13, 14]. In the model, lower NO_x are observed as the octane number is increased, this was due to a lower combustion temperature for the bulk of the 84PRF when compared to n-heptane. However this was not observed experimentally with NO_x being more constant, the sources for this error are anticipated to be associated with mixture preparation rather than the chemical model itself - however this is an area of further model refinement and improvement.

6.3 Combustion Stability

One of the major advantages of PPCI over HCCI combustion is the additional control of ignition and the rate of combustion. The results presented above highlight that a preferred fuel would have a greater resistance to ignition - however as the mixture spends more time between injection and ignition the composition becomes increasingly homogeneous. This is evident in Figure 5b with the observation that the higher octane number fuels are more homogeneous at the point of ignition. This makes fuels with increased resistance to ignition more prone to the same issues which limit HCCI engines such as combustion stability.

In an effort to characterize combustion stability, an attempt to simulate cycle-to-cycle variation was attempted. Whilst there are many potential sources of cycle-to-cycle variations, in this study the main sources were considered to be fluctuations in the pressure/temperature at IVC and the total injected fuel mass. These were varied by +/- 10% individually and in combination by carrying out a further 90 computations and examining the maximum deviations. The resulting impact of cycle-to-cycle variations are presented in Figure 6a. As an example the result from the 70PRF blend is presented in Figure 6a and Figure 6b, as observed in this case misfiring and partial burn cycles were computed with corresponding increased concentrations of uHCs and CO. This observation explains the sources of the differences in model and experiment noted in Figure 2d and Figure 2e, where a simulated mean cycle resulted in emissions much lower than observed experimentally.

In Figure 6c, the cycle-to-cycle variations with respect to octane number are presented. As octane number increases, sensitivity to cycle-to-cycle variations also increases in terms of the fluctuations of peak pressure and the total mass fraction burned. Misfire/partial com-



(a) Combustion delay (CD) and start of injection (SOI) times



Figure 5: Influence of the fuel on combustion, emissions and combustion stability







(c) Fluctuations in Mass Fraction Burned (MFB) and peak pressure

Figure 6: Cycle-to-cycle variations

bustion is computed in some of the cycles above and octane number of 70. As observed, an increased octane number results in a greater fluctuations in both peak pressure and total mass fraction burned indicating that higher octane rated fuels are more likely to suffer from issues of combustion stability and cycle-to-cycle variations. This observation demonstrates the sensitivity of PPCI combustion to "over-mixing" and highlights the associated challenges in its control.

Above an octane number of 70 in some of the cycles, partial combustion or misfire itself was computed. At a fundamental level this was considered to occur due to an increased Combustion Delay, CD rather than due to the fuel itself. For example the higher rated octane number fuels would ignite in a similar way to the lower rated octane fuels with lower sensitivity to "over-mixing" if temperature at TDC (through higher manifold pressure or increase compression ratio for example) were increased. However increased PM would be expected. This is summarized in Figure 7 where the trade-off between high PM and "over-mixing" is illustrated for varying CD.

These observations are consistent with those noted in [13, 14] where neither a conventional diesel nor gasoline standard yielded an adequate compromise balance between high PM and "over-mixing", in these cases lower octane rating gasoline fuels were considered more favorable for PPCI applications.



Figure 7: Impact of CD on PM emissions (normalized by max. computed value)

7 Discussion

For the first time, detailed chemistry and pollutant formation model have been employed with an advanced in-cylinder model to fully characterize in-cylinder stratification in PPCI engines to investigate fuel effects on PM and combustion stability. These computations have highlighted that optimal PPCI combustion is a compromise between conventional mixing controlled combustion with its associated high PM emissions, and that of kinetically controlled combustion with lower emissions but lower combustion stability. The applied model enables engineers to visualize the composition of the in-cylinder mixture with respect to crank angle and resulting simulations have demonstrated that PM is formed when there is insufficient mixing time prior to combustion, ultimately resulting in combustion in the rich regime. This can be negated by increasing the resistance of the fuel to ignition, thus allowing more mixing to occur and in a leaner mixture composition at the point of ignition. In the cases reported here, combustion is initiated in at lean equivalence ratios for the 84PRF whilst at the richest point in the n-heptane case. This enables combustion to occur whilst avoiding the high PM regime. However if longer residence times are required to ignite the mixture, ignition becomes kinetically controlled thus reducing the control over the onset of ignition and associated combustion stability issues.

For the first time using a computational model, the above results highlight that present fuel standards for conventional diesel or gasoline are insufficient to fully exploit the potential of PPCI for ultra-low PM, lower octane gasoline fuels (i.e. 84 RON) or lower cetane number diesels are required.

8 Summary

The combustion simulation tool SRM SUITE has been employed to investigate fuel effects on PPCI combustion. Three key aspects were observed;

- That SRM SUITE can be employed to successfully simulate and visualize PPCI combustion phasing and exhaust gas emissions for the full range of octane numbers.
- As octane number is increased that tendency to produce PM is reduced due to increased mixing time.
- Due to increased mixing times, sensitivity to cycle-to-cycle variations and combustion stability limits the maximum practical octane number applicable to PPCI.

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