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Simulating combustion of practical fuels and blends for modern engine applications using detailed chemical kinetics

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Abstract

This research describes the potential to adopt detailed chemical kinetics for practical and potential future fuels using *tri-component* surrogate mixtures capable of simulating fuel octane "*sensitivity*". Since the combustion characteristics of modern fuels are routinely measured using the RON and MON of the fuel, a methodology to generate detailed chemical kinetic mechanisms for these fuels based on these data is presented. Firstly, a novel correlation between various tri-component blends (comprised of i-octane, n-heptane and toluene) and fuel RON and MON was obtained by carrying out standard octane tests. Secondly, a chemical kinetic mechanism for tri-component fuels was validated using a Stochastic Reactor Model (SRM) suite, an in-cylinder engine combustion simulator, and a series of engine experiments conducted in HCCI operating mode. Thirdly, the methodology was applied to predict combustion characteristics of a practical gasoline and fuel blends with ethanol and di-iso-butylene blends using detailed chemical kinetics. Finally, for the first time the application of this technique was demonstrated by employing detailed chemistry in the optimization of two engines and two fuels operating in HCCI mode. Here a parametric study highlighted the adoption of fuels with "*sensitivity*" could significantly extend the HCCI peak operating IMEP limit by as much as 60%.

Contents

1 Introduction

Recent advances in chemical kinetics have brought about ever more robust fuel models capable of computing the combustion characteristics of the higher molecular weight hydrocarbon fuels [1–3]. However, due to the vast number of hydrocarbons blended into practical gasolines [4], surrogates representative of the fuel (usually based on a simplified alkane with equivalent carbon number) are typically adopted in order to simplify the chemistry [3]. Conventionally, these have been mono or bi-component surrogates, that is either i-octane or a Primary Reference Fuel (PRF), where the PRF is adopted in i-octane/n-heptane proportions equivalent to the RON of the practical fuel, or by subtle tuning of the blend to match with corresponding experimental data [5]. However by definition, a PRF blend has zero fuel "*sensitivity*", S = RON-MON, hence meaning it is an insufficient surrogate for fuels with "*sensitivity*". This limits the practical robustness of their adoption in a predictive sense for the full range of fuels and operating points observed in modern engines [6–8].

Critically, most practical modern-day automotive fuels do exhibit fuel "*sensitivity*", as do many of the fuels proposed for the next generation of engine technologies such as bio-/alcohol based fuels, dieseline (gasoline/diesel blends) etc. Hence, in order to facilitate engine development toward future fuel technologies, kinetic models with the ability to represent multiple fuels including those fuels with "*sensitivity*" are a fundamental necessity.

Published data on practical and commercial fuels is typically very limited. This may be due to the fuel containing multiple components, confidentiality, cost of fundamental measurement etc., hence the automotive community is often restricted to assessing combustion characteristics of the fuel by adopting the corresponding RON and MON test results [9, 10]. Whilst these tests are sensitive to many of the major fuel and combustion characteristics such as autoignition, propagating flame speed, fuel latent heat of vaporisation etc, this is usually in combination, however some insight into their nature is obtained by their acquisition. In the absence of any further information, any model of the fuel must at least have the ability to represent the RON/MON of the fuel before being applied to practical combustion problems.

When mixed in the required proportions, *tri-component* blends of i-octane, n-heptane and toluene (Toluene Reference Fuels, TRFs) have the potential to form surrogates of fuels with "*sensitivity*". However, few data are available at present in relating these with the corresponding RON/MON data [6–8]. In this study, the resulting RON and MON of various TRF blends are presented from a series of standard octane tests carried out at Shell [9, 10]. These data are used to form a correlation of corresponding RON and MON for *tri-component* blends.

Hence when applied to the reverse problem, the RON and MON can be used to determine corresponding proportions of the *tri-component* mixture, these same proportions can be employed in a chemical kinetic mechanism [2]. The *tri-component* mechanism can then be used to simulate the combustion characteristics of practical fuels with greater robustness over a range of conditions than could ever be achieved by adopting conventional mono or bi-component surrogate fuels.

A detailed mechanism for TRF blends has been proposed by Andrae et al.[2] containing 137 species and 633 reactions. However due to the size of the mechanism and the associated computational cost, it is impractical to adopt it directly into a standard multi-dimensional CFD code and solve in each grid mesh. Conversely, previous simulations of HCCI combustion using this mechanism [2] using the Homogeneous Reactor Method (HRM) have demonstrated the need to adequately characterise in-cylinder inhomogeneities, in particular in terms of stratification of the in-cylinder temperature and composition. By adopting a Stochastic Reactor Method (SRM) in-cylinder combustion simulator, these aspects are addressed resulting in improved computations of heat release profiles and exhaust gas emission concentrations (soot, CO, HC and NOx) when compared to experimental measurements [11–13].

The adopted *tri-component* chemical kinetic mechanism is used with SRM Suite and validated against a database of experimental engine data undertaken for a number of fuel blend mixtures comprised of i-octane, n-heptane and toluene over a wide range of operating conditions. The predicted in-cylinder pressure profiles are compared with measured values obtained from running single-cylinder research engines in HCCI mode [2, 7]. Next the combustion characteristics of a practical 98.5 RON and 88 MON gasoline fuel, ethanol and di-iso-butylene - PRF blends are simulated in HCCI mode using a TRF surrogate fuel generated directly from the fuel RON and MON. Corresponding results and shortcomings of the methodology are discussed.

Finally, the influence of fuel "*sensitivity*" on the HCCI operating window was examined at two representative operating points by increasing the fuel concentration to obtain the knock limits for two fuel surrogates. The results demonstrate the impact of fuel sensitivity on extending the high load limit of HCCI engine combustion.

2 Tri-Component Surrogate Fuel Generation

In order to equate the corresponding range of Research and Motor Octane Numbers associated with various blends of i-octane/ n-heptane and toluene, a series of RON/MON experimental tests were conducted by Shell for various *tri-component* blends. The procedure for these tests are outlined elsewhere [9, 10].

Standard tests were carried out for the fuel blends and these are outlined in Table 1, the design matrix conformed to an augmented simplex experimental design. These data were then used to equate RON and MON for all TRF blends using a 2nd order response surface regression technique. Known values of RON/MON for PRFs, toluene and measurements published elsewhere [2, 7, 8] were used for further validation of the correlation. The resulting correlation, presented in Figures 1(a) and (b), are ternary plots of RON and "*sensitivity*" respectively in the *tri-component* mixture space of the toluene/i-octane/n-heptane blends.

Each axis of the diagram represents a volume fraction of n-heptane, toluene and i-octane. By tracing lines inward to the intercept of these three components, the RON or MON can be obtained. It is interesting to note the octane number and "*sensitivity*" do not blend linearly, i.e. the contours of constant RON or "*sensitivity*" show curvature. This is most

Table 1: *Experimental design matrix and results for TRF fuel testing*

toluene (vol. %)	i-octane (vol. %)	n-heptane (vol. %)	RON	MON
100.00	0.00	0.00	120.0	109.0
66.66	16.66	16.66	98.0	87.4
50.00	50.00	0.00	110.0	99.3
50.00	0.00	50.00	65.9	57.7
33.33	33.33	33.33	76.2	70.9
16.66	66.66	16.66	87.0	84.0
16.66	16.66	66.66	39.0	37.0
0.00	100.00	0.00	100.0	100.0
0.00	50.00	50.00	50.0	50.0
0.00	0.00	100.00	0.0	0.0

Table 2: *Engine details*

	Engine A	Engine B	Engine C
Compression Ratio	16.7	14.0	22.4
Bore (mm)	127	86	121
Stroke (mm)	154	86	140
Con-rod (mm)	255	143.5	260
IVC (bTDC)	139	108	

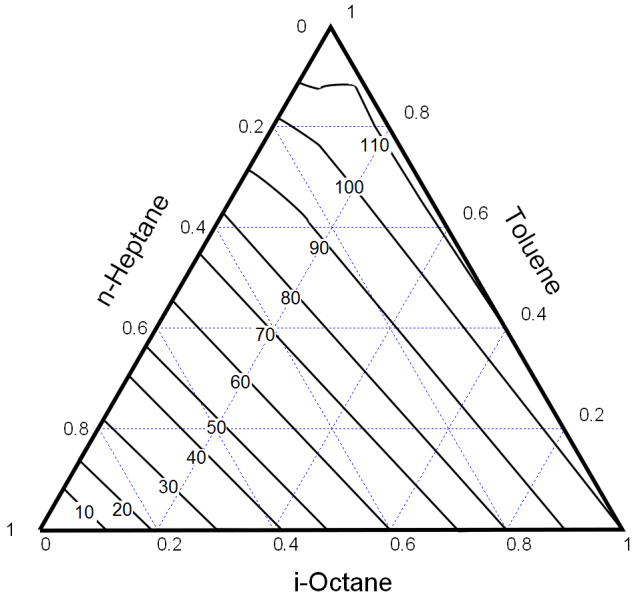
evident, in the fuel "*sensitivity*" diagram but also at the highest RON values. Whilst much of the diagram could be considered linear - the most relevant region to modern commercial fuels in terms of RON and MON (90-100 RON, $\approx$ 10 "*sensitivity*") is in the non-linear region. This suggests that conventional linear blending methods are prone to significant error and demonstrates the importance of the adopted experimental efforts and employed methodology [14].

3 Mechanism Validation

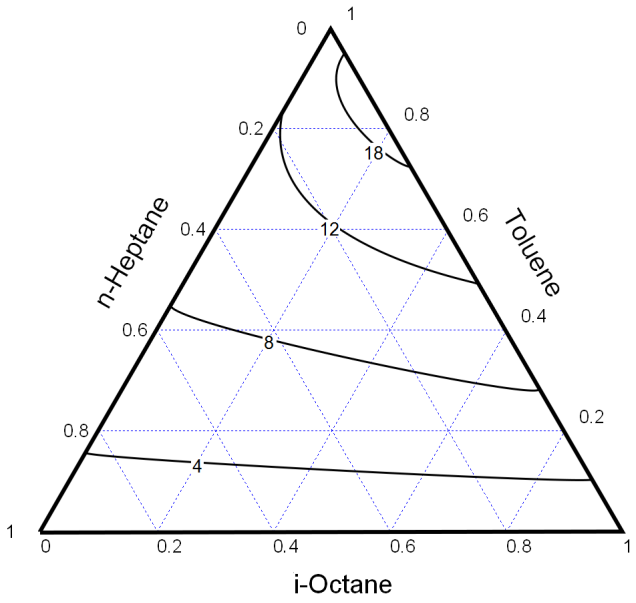
3.1 Experiments

Experiments simulated in this study are summarised as follows but are described in detail in references [2, 7, 8]. The key details of the adopted engines are presented in Table 2.

In order to simplify and isolate the influence of fuel type and in particular the impact of chemistry over and above other potentially critical engine process (such as injection, fuel stratification, flame propagation etc.) these engines were operated in HCCI mode with an early fuel injection time such that the air/fuel mixture composition could be considered well mixed and homogenous at the start of the computation.



(a) Research Octane Number (RON)



(b) Octane "*sensitivity*" (RON - MON)

Figure 1: *Ternary plots in toluene/i-octane/n-heptane mixture space*

Table 3: *Engine operating points*

	Engine	RPM	T_{IVC} (deg C)	P_{IVC} (bar)	λ
OP1	A	900	40	2.0	4
OP2	A	1200	40	2.0	5.5
OP3	A	900	120	1.0	3.5
OP4	A	1200	120	1.0	3
OP5	B	1200	250	1.0	3.5
OP6	B	1200	250	1.0	4.0
OP7	B	1200	80	2.0	4.0

3.2 Operating Points

During the process of mechanism validation, a total of seven operating conditions (see Table 3) were examined for each fuel (see Table 4), a total matrix of 26 points. The pressure-temperature histories of the unburned gas during compression up to the onset of ignition and associated with these seven operating points were considered representative of commercial naturally aspirated and turbo-charged S.I. engines [6, 15]. Furthermore, these operating points proved sufficient in demonstrating the increased or decreased relative Octane Number (Octane Index, OI) trends often reported in context with HCCI/practical fuel studies to examine fuel and engine matching [6–8]. However, more fundamentally the trends could be considered in terms of the corresponding pressure and temperature histories [6].

3.3 Engine Modeling

The stochastic reactor model (SRM) employed in this study is outlined comprehensively including a detailed mathematical description in papers [11–13]. However in this work, the code has not been developed and is only used as a tool hence the model is only described briefly here. The SRM is now a well established tool for computing engine combustion events and emissions with an history of successful validation in a number of engine related applications and results published in a large number of research articles [11–14, 16–22]. It has been successfully employed in a number of earlier studies such as port fuel injected HCCI combustion [11, 12], alternative fuel blends [13, 14], single early direct injection HCCI [16], dual injection HCCI [17], multi-cycle transient simulation and control [18–20], soot formation [21], and has been coupled to the Computational Fluid Dynamics (CFD) code KIVA [22].

The SRM is derived from more general probability density transport models (PDF) and is a zero dimensional model with statistical homogeneity assumed. This is of fundamental importance to delivering robust computations of heat release rates and emissions where inhomogeneities are critical particularly in the mixture composition and thermal domains. The model is solved by adopting a user defined number of stochastic particles which can be used to represent the PDF. These particles are not to be confused with physical atoms

Table 4: *Key model parameters*

Model parameter	value	source
Stochastic heat transfer coefficient [-]	20.0	[11–14, 16–22]
Turbulent mixing time [s]	0.005	[24]
Initial pressure/temperatures	experiment	[2, 7, 8]
Timestep [CAD]	0.2	[25]
No. of Stochastic Particles	100	[25]

or molecules, but as an ensemble constitute a statistical representation of the PDF of the in-cylinder mixture. Engine-related processes such as fuel injection, chemical kinetics, turbulent mixing, piston movement and convective wall to fluid and fluid to fluid heat transfer are solved for each stochastic particle. The greater the number of adopted particles, the finer the resolution but of course at greater computational cost. This trade-off enables the solution of interacting detailed chemical and physical processes at reduced computational cost compared to equivalent CFD approaches.

The adopted *tri-component* chemical kinetics were based on an toluene/ n-heptane/ i-octane oxidation mechanism [2] which was comprised 137 species and has previously been optimised and validated against ignition delay times from shock tubes and rapid compression machines, observed flame speeds from counter-flow flames and HCCI engine ignition timings.

In this study, the SRM was applied to simulate the closed volume portion of the engine cycle, i.e. from IVC to EVO. Presented in Table 4 are a summary of the key model parameters adopted here. Given the large number of parameters required in any engine model particular when detailed fuel models are employed, it is of extreme importance to deliver validation exercises against data from a variety of sources, engines and operating points. Particularly when considering the observations outlined in [6–8], where alternative pressure and temperature histories have been proven to be so critical in studying fuels with sensitivity. Of equal importance is the impact of the initial set of model parameters employed by the model - to be truly robust these parameters must be fixed or modified in a logical way with full justification. In this study, model parameters remained fixed throughout whilst the initial pressure and temperatures were determined according to the experimental data for each operating point. Once determined, the simulations were completed for each corresponding fuel taking up to sixty minutes using a standard desktop PC. Further details of these aspects should be obtained from our previous publications [15, 23].

3.4 Results

The model and experimental pressure-crank angle data at Operating Points (OP) 1 and 7 are presented in Figure 2. In these cases, the pressure due to compression and expansion prior to and well after ignition are sufficiently within any reasonable accepted experimental and modeling uncertainties. These results proved typical across many of the simulations, as ignition onset times and subsequent heat release rates were largely predicted well. Presented in Table 6 is a summary of the experimental, simulated and observed

Table 5: *Fuel blends adopted in this study*

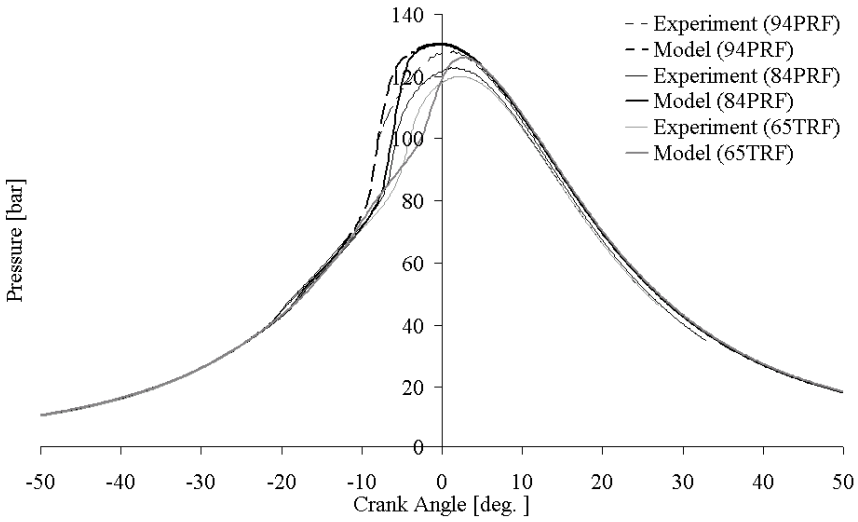
Fuel	i-octane (%vol)	n-heptane (%vol)	toluene (%vol)	other (%vol)	RON	MON
94PRF	94	6	0	0	94	94
84PRF	84	16	0	0	84	84
75TRF	0	25	75	0	94.2	82.6
65TRF	0	35	65	0	83.9	73.2
62TRF	0	38	62	0	80.5	70.3
50TRF	0	50	50	0	64.1	58.1
Surrogate A	63	17	20	0	88	85
Surrogate B	69	17	14	0	87	85
98ULG	0	0	0	100 (ULG)	98.5	88
65PRF/ethanol	52	28	0	20 (ethanol)	86.9	83.6
57.3PRF/di-iso-butylene	43	32	0	25 (di-iso-butylene)	83	78.9

model error for the crank angle at 50% heat release. Generally, most operating points were simulated to an accuracy of within ± 2 CAD with the trends of the experimental data were also observed in the model results. Finally, when adopted as a *tri-component* mixture (surrogate fuel blends) at OP6 and OP7, the mechanism and model performed very well, hence the *tri-component* fuel mechanism plugged in the SRM suite was considered as an adequate tool for further model application.

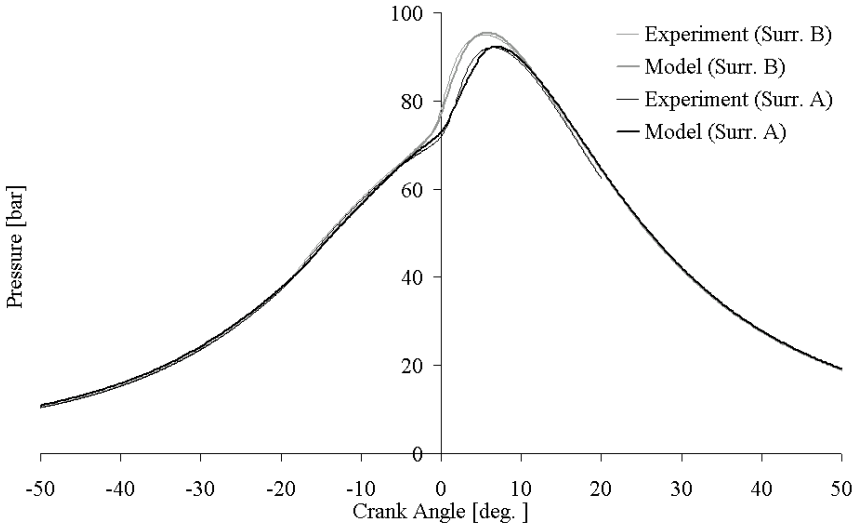
The major aspects requiring further consideration were the results relevant to the 75 TRF, for OP 1 and 2 where no ignition was reported, here some combustion was predicted by the model, however in both cases the actual total heat release proved trivial and as such these computations were considered to be misfired events. However, at OP 3 and 4, the computations of the 75 TRF blend demonstrated to have the poorest performance noted in the study. However, it was concluded that by coupling the model properly with a 1D engine cycle model, a better estimate of the conditions at IVC that is considering charge cooling, engine breathing etc. could well be expected especially given that this fuel yielded the latest ignition time, hence assumptions of identical EGR and initial temperature across all these fuels may well not be appropriate in these cases. The authors do consider the reliability of the reaction rate parameters for the toluene oxidation component of the mechanism may well be a possible source of this inaccuracy. However given the success of the mechanism for the other fuel types further refinement of the mechanism was considered unjustified here without an equally detailed consideration of the boundary conditions of the in-cylinder model. Hence, the mechanism was considered robust enough to be adopted in further examination of fuel and engine parametric and validation studies.

4 Modeling Fuel Octane "*Sensitivity*"

Since the vast majority of engines are operated using commercial fuels, a chemical kinetic mechanism for these fuels is prerequisite for the development of more robust in-cylinder



(a) Operating Point 1



(b) Operation Point 7

Figure 2: *Pressure vs. crank angle for experiment and model. Experimental uncertainty is expected to be* ± 1.0 *bar at TDC and* ± 0.2 *crank angle degrees*

Table 6: *Summary of model results in Crank Angle Degrees for 50% heat release with experimental uncertainty of 1.0 Crank Angle Degree*

	Fuel	Experiment	Model	Error
OP1	94PRF	-5.6	-6.2	0.6
	84PRF	-8.0	-8.1	0.1
	75TRF	No ignition	5.9 (low H.R.)	-
	65TRF	-3.5	-1.7	1.8
	62TRF	-4.6	-3.2	1.4
OP2	94PRF	-5.1	-6.7	1.6
	84PRF	-7.2	-8.2	1.0
	75TRF	No ignition	1.4 (low H.R.)	-
	65TRF	-2.4	-0.8	1.6
	62TRF	-3.9	-2.2	1.7
OP3	94PRF	7.4	0.6	6.8
	84PRF	-4.3	-4.1	0.2
	75TRF	4.9	-0.9	5.8
	65TRF	-4.2	-4.7	0.5
	62TRF	-5.7	-5.7	¡0.1
OP4	94PRF	8.0	6.4	1.6
	84PRF	-2.4	-0.5	1.9
	75TRF	7.3	0.2	7.1
	65TRF	-4.0	-3.8	0.2
	62TRF	-5.4	-4.8	0.6
OP5	64TRF	0.2	-4.8	5.0
	50TRF	-6.0	-8.0	2.0
OP6	Surrogate A	-0.1	-0.2	0.1
	Surrogate B	0.1	0.2	0.1
OP7	Surrogate A	3.0	3.2	0.2
	Surrogate B	2.0	1.7	0.3

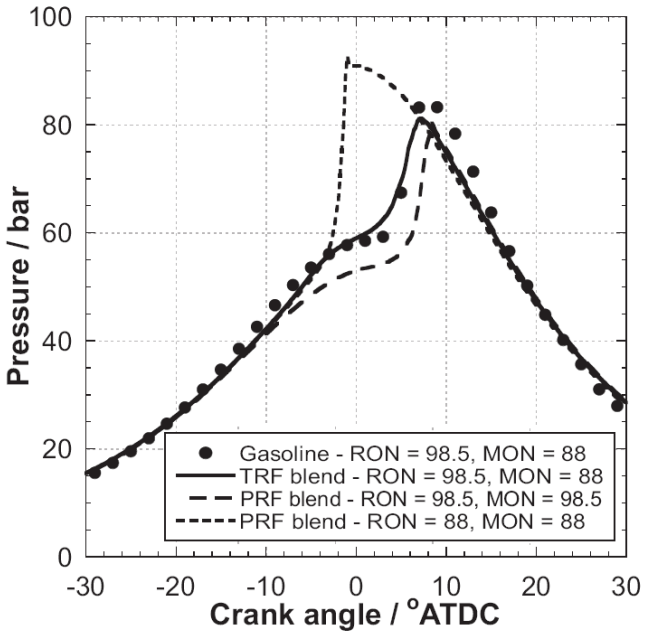


Figure 3: *Pressure curves for the HCCI engine experiment with commercial gasoline*

combustion simulations. Given the complexity of these fuels in terms of their (varying) composition and the lack of fundamental measurements which can be used to map out the key combustion characteristics, only a limited amount of data are available to development engineers. As such in this research, a surrogate of a commercial gasoline was generated based on a RON of 98.5 and its corresponding MON of 88. Using these data and the ternary plots, a surrogate TRF fuel of composition 75.4% toluene, 5.8% i-octane and 18.8% n-heptane was generated. This composition was adopted to simulate the fuel in a variable compression ratio engine, Engine C at a number of operating conditions. Details of this study are reported in more detail elsewhere [15, 23] but are summarised in Figure 3.

In this case, three fuel surrogates were generated, the *tri-component* surrogate based on the methodology outlined in this research, a PRF based on the RON and a PRF based on the MON. In this case, the 88 PRF proved to ignite too early and the 98.5 PRF far too late compared to the experiment, however the *tri-component* surrogate proved to be adequate for representing the combustion characteristics of the commercial gasoline.

This result demonstrates the clear added value of employing this methodology over equivalent conventional *mono* or *bi-component* surrogate methods.

4.1 Bio-Fuel/Gasoline Fuel Blends

Due to the time and costs associated with chemical kinetic model development, unique blends of fuels are unlikely to have a corresponding chemical kinetic mechanism in the near future, as such the proposed methodology can be used effectively to determine an equivalent surrogate fuel for adoption in computational modeling. In an effort to test the scope of this methodology in computing the equivalent combustion characteristics, the

Table 7: *Summary of model results in Crank Angle Degrees for 50% heat release with experimental uncertainty of 1.0 Crank Angle Degree*

	Fuel	Experiment	Model	Error
OP1	57.3PRF/di-iso-butylene	-8.3	-7.8	0.5
	65PRF/ethanol	-6.1	-6.3	0.2
OP2	57.3PRF/di-iso-butylene	-7.2	-7.9	0.7
	65PRF/ethanol	-5.8	-6.5	0.7
OP3	57.3PRF/di-iso-butylene	-3.8	-6.6	2.9
	65PRF/ethanol	-0.9	-3.4	2.5
OP4	57.3PRF/di-iso-butylene	-3.2	-4.9	1.7
	65PRF/ethanol	0.2	-1.6	1.8

same methodology was applied to examine two further fuel blends.

Using the RON, MON measured by Shell and the ternary plots presented in Figure 1, a blend of 17% n-heptane, 63% i-octane and 20% toluene was used as a surrogate of the 65PRF/ethanol fuel blend and a second blend of 27% n-heptane, 50% i-octane and 23% toluene was formed as a surrogate the 57.3PRF/di-iso-butylene mixture.

Simulations were setup with identical boundary conditions to those outlined in the previous sections. Presented in Table 7 are the corresponding results of these simulations. In most cases, the model error was less than two crank angle degrees which demonstrates the potential of the methodology for further development and its potential to yield reliable representative combustion characteristics for a wide range of practical fuels and blends.

4.2 High Load Knock Limit

The operating window of an HCCI engine is a major area of interest in developing the mode into a low emission, high fuel economy and practical technology. The high load operating point is of particular interest as it reaches a practical limit caused by the onset of HCCI engine "knock". That is, an overly rapid heat release rate which results in an undesirable in-cylinder "pinging" noise and in the long term, associated engine damage [24, 26]. It was felt that a parametric study of the influence of fuel sensitivity on the knock limit would form an ideal application of employing the proposed methodology to a practical problem - that is using detailed chemical kinetics to optimise maximum engine performance characteristics across a range of engine speeds.

In order to examine the influence of fuel sensitivity on the high load operating limit of Engine A, a series of parametric sweeps were carried out for Operating Points 2 and 4. These two Operating Points were selected as representative of the typical P-T-t histories of an exaggerated turbocharged (with intercooler) (TC) and a naturally aspirated (NA) engine, respectively. To simulate an increasing engine load, the in-cylinder fuel concentration was increased. A 94 PRF and a 75 TRF (94.2 RON 82.6 MON) fuel were adopted for the study of sensitivity as they represented a sensitivity of 0 and 11.6 respectively. In total over one hundred engine cycles were simulated for each fuel at a range of engine speeds and equivalence ratios taking around 400 computational hours. In order to reduce

the number of computations, it is important to note that the concentration of EGR was not varied in this exercise and in principle could be employed successfully to further extend the operating window.

The maximum IMEP was constrained by limiting the 50% heat release rate to after TDC and estimating HCCI engine "knock" as a maximum value of dp/dt, whilst a clear definition of this value appear to be engine dependent [26, 27], it was considered here to be of the order of 100 bar/ms.

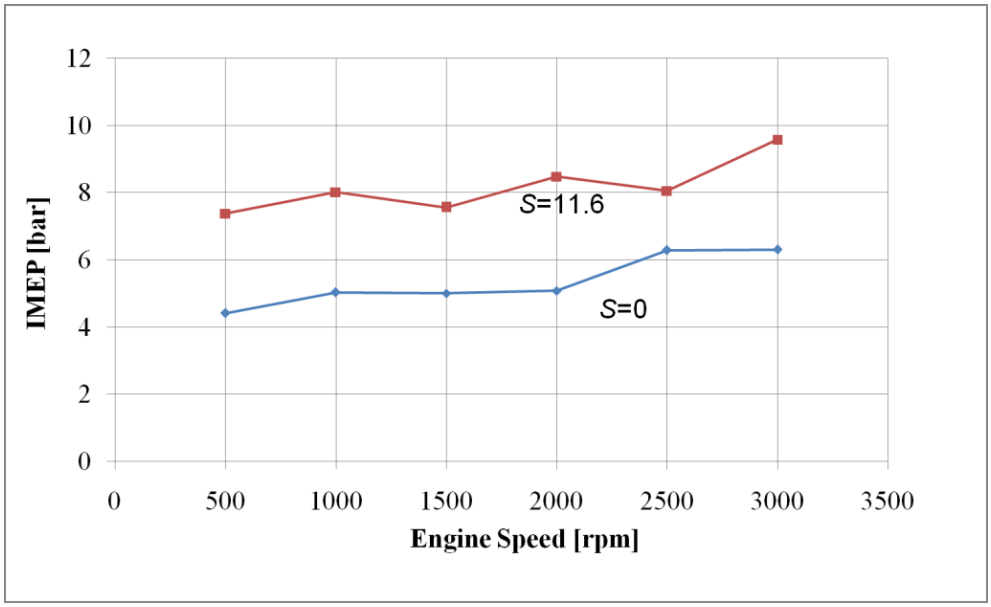
Presented in Figure 4 are the resulting maximum IMEP for the TC and NA engines for a range of speeds. In the TC engine, the fuel with "*sensitivity*" yielded greater IMEP for a given speed than the fuel without. This was in simple terms, because the peak non-knocking IMEP was achieved with an equivalence ratio of 0.25 and 0.15 respectively, yielding a significant 60% increase in the achievable load. For the NA engine, at low engine speed the fuel with zero sensitivity yielded greatest IMEP, then at 2000 RPM and greater, misfire was reported. This was due to a shortened residence time during compression, conversely the fuel with sensitivity ignited at all engine speeds.

These computations compare well with equivalent experimental observations and empirical analysis of fuels with and without sensitivity by Kalghatgi et al. [8] and more recently the work of Shibata and Urushihara [28–30]. The latter propose that fuels with sensitivity have a duel phase high temperature heat release, which results in a longer combustion duration.

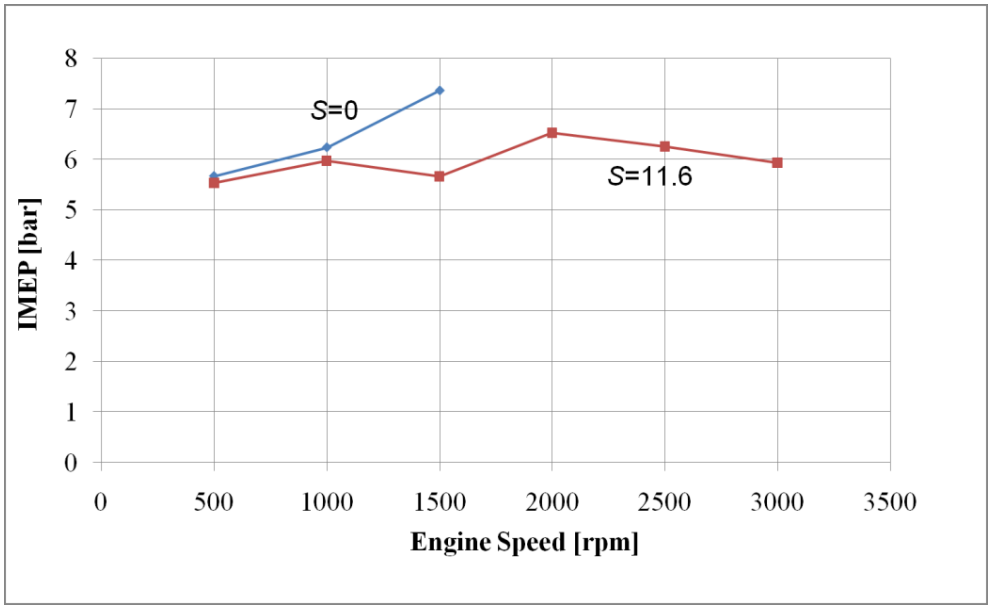
These model results demonstrate these same aspects can now be simulated indicating that fuel sensitivity can be exploited to extend the peak load operating points based upon the lengthening of the combustion duration for a given stratification. Presented in Figure 5 is an example of how the two fuels compared during a number of combustion events with increasing equivalence ratio, if ignition occurred at approximately the same time (Start of Combustion, 10% heat release), the fuel with sensitivity tended to have a longer combustion duration resulting in a lower dp/dt and thus "knock" tendency. This allowed for the engine to be operated at greater equivalence ratios and loads. Since, the in-cylinder spatial temperature distribution for both the fuels could be considered similar prior to ignition, this suggested that the "sensitive" fuel is influenced more by the same temperature distribution, resulting in a larger distribution of ignition delay times within the cylinder. That is, by having a larger variation in ignition delay times, as demonstrated in the NA engine, these fuels are also potentially easier to ignite and once ignited, the subsequent pressure and temperature increases due to heat release are sufficient to complete the combustion over a longer duration. Hence this indicates that fuels influenced most by spatial in-cylinder temperature, are ideal for extending the maximum HCCI operating limit.

5 Discussion

The presented methodology proposes a *tri-component* blend as a surrogate for practical gasoline using standard fuel metrics - the road- and motor- octane numbers - to dictate the composition. The example case of a 98.5 RON gasoline is that of a relatively high quality fuel, however equivalent blends can be formed for standard European gasolines and the



(a) Turbocharged (with intercooling) limit



(b) Naturally aspirated limit

Figure 4: *Engine Speed versus IMEP*

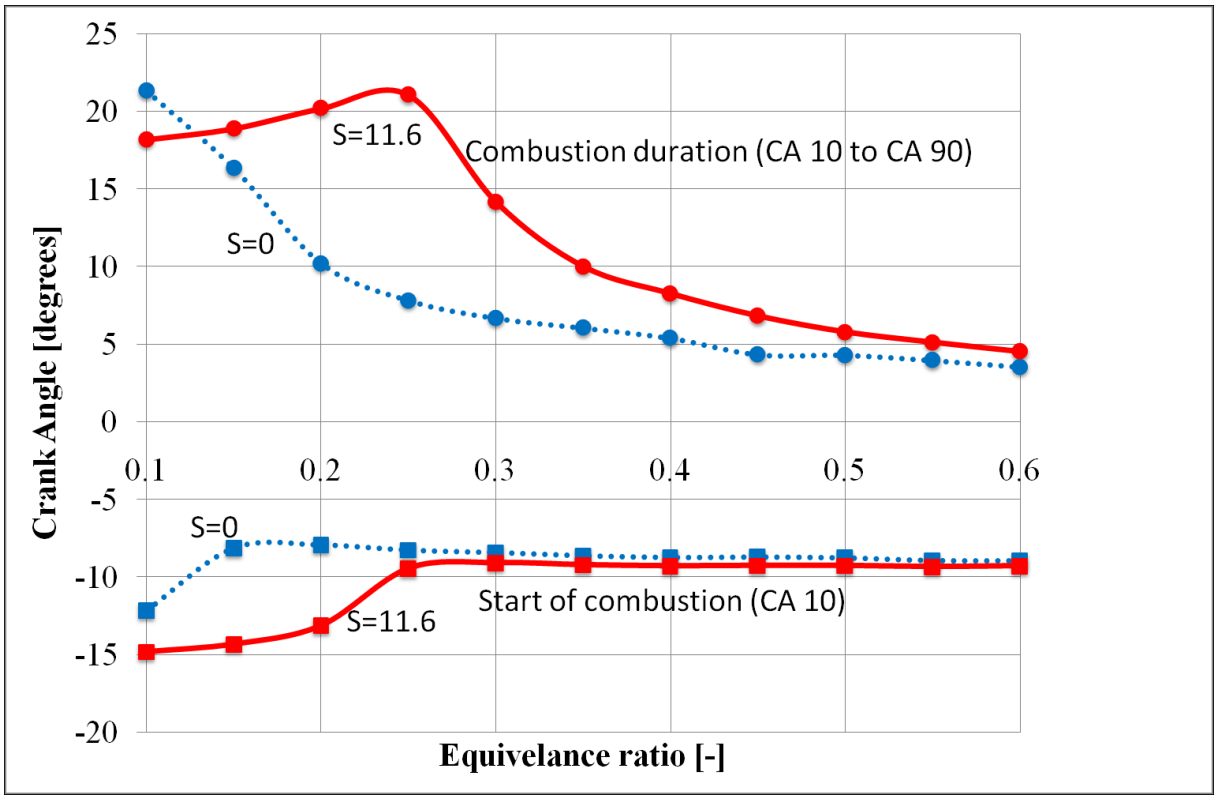


Figure 5: *Equivalence ratio versus the start of combustion and combustion duration for fuel with and without sensitivity at Operating Point 2 and 2000 rpm.*

"cheaper" grades of gasolines. By mapping the RON and MON for different TRF fuel blends, engineers now have, for the first time, the ability to model different fuel grades and blends of fuel as long as octane numbers are known. This also presents an opportunity for the simultaneous development of an engine and fuel together via computational modeling - a task of particular interest to those examining Premixed Charged Compression Ignition technologies where gasolines and blends of gasoline and diesel with lower RONs and MONs are proving more appropriate [31].

This technique links to the fundamentals of chemical kinetic mechanism development via the adoption of a Stochastic Reactor Model (SRM) in-cylinder combustion simulator. By eliminating the complex engine combustion flow processes (adequate for HCCI) but still retaining mixture strength- and temperature- stratification, the full benefits of detailed mechanisms can now be exploited properly by the automotive community. Benefits including improved robustness in terms of heat release rate and emissions calculations. Critically, when compared to conventional CFD, computations are completed in timescales, which are amenable to carry out optimisation and parametric studies. The latter are of particular importance when seeking subtle efficiency gains in engine performance for "blue-sky" development phases of projects such as searching for ideal fueling choice and strategy.

The RON/MON test data have highlighted a number of interesting observations which require further consideration. Firstly, the fact that TRFs do not blend in a linear manner is critical when employing this sort of methodology as small deviations in the calculation of RON and MON can lead to significantly different engine performance. This justifies these experimental research efforts, and demonstrates its importance when considering the adoption of *tri-component* surrogate fuel models.

The requirement for non-linear blending correlations highlights a secondary aspect when considering the reverse problem employed in this paper. That for a limited number of *tri-component* mixtures there may be more than one TRF blend for a given corresponding RON and MON. Unfortunately in this research there was no relevant experimental data available for these cases thus it was not possible to investigate this any further. However, under such circumstances it is suggested that other fuel properties should be identified such as laminar flame speed or aromatic composition, which enable engineers to identify a unique blend.

One major aspect of the adoption of chemical kinetics into engine simulations is the increased capability of delivering improved emissions analysis. Whilst it is fundamental for robust emissions models to be preceded by a robust combustion model, emissions are also linked to the composition of the fuel, for example soot is promoted in fuels with aromatic rings [24]. Hence the adoption of this methodology is, at present most applicable for determining combustion characteristics such as heat release rates and corresponding emission computations cannot be considered as reliable as might be expected from a kinetic mechanism developed specifically for the employed fuel and fuel blend. Clearly, the presented technique should never be used as a replacement for a formal chemical kinetic mechanism of the oxidation of the adopted fuel or fuel blend but only serves as a generic method to deliver the levels of robustness associated with the adoption of detailed chemical kinetics in computational modeling to complex practical fuel blends such as gasoline.

The example of generating a surrogate for the 98.5 RON commercial gasoline and the parametric study of the peak IMEP operating limit of HCCI engine, highlight the dangers associated with using an inadequate bi-component surrogate fuels. In both cases, significant differences in performance characteristics were noted in surrogates with and without sensitivity, indeed the maximum IMEP yielded a 60% difference. This result highlighted the importance that stratification has on preventing "knock" and increasing the peak IMEP limit. Stratification is conventionally considered to be controlled by heat transfer, mixing and the injection strategy, whereas in principle - even more significant results could be achieved by exaggerating these same aspects using intelligent fuel design. Indeed these same aspects have been reported in experimental studies for HCCI engines [8, 28–30]. That is adopting fuels most sensitive to fuel and temperature stratification in terms of their propensity to autoignite, hence reduced heat release rates for a given fueling rate and therefore higher loads can be achieved.

6 Conclusions

Often the only combustion characteristics available for practical fuels are the fuel RON and MON, hence a new method to generate *tri-component* surrogate blends based on these metrics was outlined.

Firstly, a chemical kinetic mechanism for *tri-component* blends was implemented into a Stochastic Reactor Model (SRM) suite and the mechanism successfully validated against experimental data for a variety of *tri-component* blended fuels and operating conditions. A series of RON and MON tests were conducted to correlate the *tri-component* blend composition against corresponding RON and MON, these results demonstrated that non-linear mixing blending laws are required for the proper adoption of these methods.

This methodology was demonstrated as a promising technique for determining combustion characteristics of practical gasolines and fuel blends by carrying out successful simulations of a practical 98.5 RON/88 MON gasoline and ethanol and di-iso-butylene blends.

Results indicated significantly improved performance for examining practical fuels and fuel blends when compared to *mono* or *bi-component* fuel surrogates.

Finally, for the first time, detailed chemical kinetics were employed to determine the peak load operating limit with respect to engine speed of two engines operating in HCCI mode with and without fuel sensitivity. Results demonstrated that octane "*sensitivity*" could be exploited for future fuel design in order to extend the HCCI operating window.

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