Role of Fuel Sensitivity in Extending the HCCI Engine Operating Window

Andrew Smallbone, Amit Bhave
Reaction Engineering Solutions Ltd, Cambridge, U.K.

Neal Morgan, Markus Kraft
Department of Chemical Engineering, University of Cambridge, Cambridge, U.K.

Roger Cracknell, Gautam Kalghatgi
Shell Global Solutions, Chester, U.K.

Summary

Despite the ultra-low NO_x and soot emissions associated with HCCI engine technology, the operating window of an HCCI engine is narrow and is limited by knock on the high load side. We apply a probability density function (PDF) based stochastic reactor model (SRM) to investigate the role of fuel sensitivity in expanding the HCCI operating range. Toluene Reference fuels (TRFs) – a tertiary mixture of Toluene, n-Heptane and iso-Octane exhibit higher sensitivities than primary reference fuel (PRF – zero sensitivity), and can be considered closer to real gasoline fuels. A detailed TRF chemical mechanism comprising 137 chemical species and 633 reactions is incorporated in the SRM. The SRM accounts for the inhomogeneities in temperature and composition arising due to fuel injection, turbulent mixing and heat transfer between hot charge and cold cylinder walls. The model is validated against experiments published by Kalghatgi et al. [SAE 2003-01-1816] and Andrae et. al. [Combust Flame, 2008], in which PRFs and TRFs were used in single cylinder HCCI research engines. The validated model is then applied at high load points and the influence of fuel sensitivity on the reported Mean Effective Pressure (MEP) is discussed.

1. Introduction

In the standard RON (Research Octane Number) and MON (Motor Octane Number) tests, practical fuels are matched to PRF (Primary Reference Fuel) blends of n-heptane and iso-octane which exhibit similar anti-knock tendencies [1, 2]. Fuel "sensitivity" is defined as the difference between the (RON-MON) octane numbers. For example, a standard gasoline in the EU is approximately a 95.3 RON and 85.3 MON rated fuel with a sensitivity of 12 [3]. In physical terms, this fuel when exposed to the pressure-temperature history at the RON operating point, had the equivalent anti-knock properties of a 95.3 PRF and equivalent to a 85.3 PRF at the MON operating point. Hence, depending on the imposed pressure-temperature history, a fuel with "sensitivity" is only directly relevant to the RON/MON PRF equivalents at the RON and MON Operating Points (OPs) themselves [3,4,5].

Such observations, were demonstrated in HCCI [4] and SI combustion [5] for various fuels with sensitivity. These observations have led to the adoption of an Octane Index, *OI*.

$$OI = (1-K)(RON) + K(MON)$$

Where *K* is a constant representative of the pressure-temperature history. Correlations have been developed in terms of the in-cylinder temperature at an in-cylinder pressure of 15 bar [5]. In simple terms, *K*=1 at the MON operating point and *K*=0 at the RON operating point. A fuel with *positive K* and fuel "sensitivity" would be expected to have an octane index, *OI*< RON and *OI*>RON for *negative K*. Hence, a fuel with "sensitivity" in an engine with a particularly high end gas pressure for a given temperature (e.g. turbocharged engine with intercooler) would expect to have a greater resistance to knock than the equivalent PRF.

Recent advances in chemical kinetics have yielded larger and ever more reliable fuel models capable of representing autoignition and flame propagation of the higher molecular weight hydrocarbon fuels [6, 7, 8]. However, due to the vast number of hydrocarbons blended into practical gasolines [9], a surrogate fuel representative of the properties of that fuel, usually based on a simplified alkane with equivalent carbon number was typically adopted in order to simplify the chemistry [8]. Traditionally, this surrogate was either iso-octane or a PRF, where the PRF was adopted in proportions equivalent to the RON of the practical fuel or by subtle tuning of the blend to match with the experimental data [10]. However as outlined, by definition due to fuel "sensitivity", a single PRF blend is unable to properly represent a fuel with sensitivity over the full range of operating points and engines.

In order to deal with these aspects, a detailed mechanism for TRF (Toluene Reference Fuel) blends of iso-octane, n-heptane and toluene has been proposed by Andrae et al. [7] containing 137 species and 633 reactions. Due to the intrinsic sensitivity of toluene (120 RON 109MON [11]), one is now in the position to

examine the influence of fuel sensitivity within fuel blends. However due to the size of the mechanism and associated computational cost, it is impractical to adopt it directly into a standard multi-dimensional CFD code. Conversely, previous simulations of HCCI combustion with this mechanism [7] using the Homogeneous Reactor Method (HRM) have demonstrated the need to characterise in-cylinder inhomogeneities, in particular in terms of stratification of the in-cylinder temperature and composition.

The probability density function (PDF)-based stochastic reactor model (SRM) considers detailed chemical kinetics (crucial for simulating advanced combustion modes) and accounts for inhomogeneities in composition and temperature arising from direct injection, convective heat loss and turbulent micro-mixing. The SRM coupled with a 1D engine cycle simulator is capable of modelling the combustion and emissions during closed volume period of the cycle (combustion, TDC and negative valve overlap) over manageable timescales compared to an equivalent multi-dimensional CFD code, whilst describing the non-homogenous mixture in terms of temperature and mixture strength reasonably well. Furthermore, heat release profiles and in particular the associated emissions (CO, uHCs etc.) can be predicted more accurately than if using a more conventional approach of the standard HRM [12].

Presented in this work are an examination and verification of the application of the TRF mechanism using an SRM. The predicted auto-ignition times and in-cylinder pressure profiles are compared with measured values obtained from running the single cylinder research engines in HCCI mode [4, 7]. These experiments were undertaken for a number of fuel blend mixtures comprised of iso-octane, n-heptane and toluene over a wide range of operating conditions.

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 partial burn and knock limits for two potential surrogates for standard gasoline, a 94 PRF and a 75 TRF with 94.2 RON and 82.6 MON.

2. Experimental data

Experiments simulated in this study are summarised as follows and have been described in detail in references [1] and [2]. The key details of the adopted engines are presented in Table A. Each engine was operated in HCCI mode and fuel-air mixing was considered to have occurred far enough upstream that the mixture was assumed fully evaporated and homogonous in strength.

	Engine A	Engine B
CR	16.7	14.04
Bore (mm)	127	86
Stroke (mm)	154	86
Con rod (mm)	255	143.5
IVC (bTDC)	139	108

Table A: Engine details

2.1 Operating points

In this study, a total of seven operating conditions were examined and the data are outlined in Table B. The pressure-temperature histories of the unburned gas during compression up to the onset of ignition and associated with these seven operating points are presented in Fig. 1. For comparison, equivalent data for the RON and MON tests in a turbocharged 1.4 litre VW engine and a Ford 2.0 litre naturally aspirated SI engine are also presented [3].

Table B: Engine operating points

	Engine	**RPM**	**Tin (deg C)**	**Pin (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

Operating points were selected on the basis of being representative of the full range of histories observed in both SI mode and in the definition of the RON and MON test procedures.

As presented in Fig. 1, for a given pressure, the turbocharged engine exhibited a lower end-gas temperature whereas the reverse was noted for the naturally aspirated engine. Such a diagram demonstrates that, in practice ignition can occur in regimes associated with low, intermediate or high temperature autoignition chemistry [13]. The p-T histories often passed through a number of regimes and for different time durations, as such any adopted kinetic mechanism should be able to sufficiently predict the chemistry within each regime and their interactions. It was felt that the approach adopted in this study was a more robust examination of the mechanism than achieved by simply adopting a limited number of operating points. However it is noted that ignition at all the Operating Points occurred at higher temperatures than the S.I. engine p-T histories outlined in Fig. 1 and was thus most sensitive to the high temperature regime.

2.2 Adopted fuels

The fuels adopted in this study are presented in Table C. A 75 TRF blend was selected on the basis that the corresponding RON and MON are of similar magnitude to a standard unleaded gasoline fuel in the EU [3]. As such, this blend could well be adopted to form a successful surrogate for practical gasoline. The 94 and 84 PRFs blends were adopted as they have a similar RON and MON respectively to the 75 TRF blend. The 65, 64, 63 and 50 TRF blends were adopted for thorough examination of the effects of fuel sensitivity. Finally, the Surrogates A and B were used to test whether the mechanism could predict the performance of blends comprised of all three components.

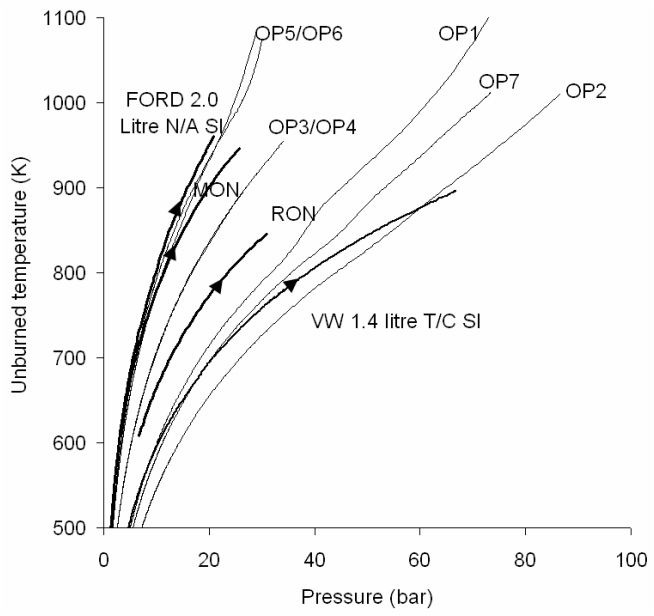


Fig. 1: Pressure-temperature histories of the adopted operating points (OPs) relative to the RON and MON test conditions, a naturally aspirated 2.0 litre Ford and a turbocharged 1.4 litre VW production engine.

4.0 Engine simulations

The SRM was applied to simulate the closed volume portion of the engine cycle, i.e. from IVC to EVO. This section summarises the boundary conditions and the fuel model used. Detailed description of the SRM approach and several studies demonstrating the application of the SRM to simulate HCCI combustion, emissions and engine performance have been published previously [14].

Table C: Fuel blends adopted in this study

	Iso-octane (%vol)	n-heptane (%vol)	Toluene (%vol)	RON	MON
94PRF	94	6	0	94	94
84PRF	84	16	0	84	84
75TRF	0	25	75	94.2	82.6
65TRF	0	35	65	83.9	73.2
64TRF	0	36	64	82.3	73.1
62TRF	0	38	62	80.5	70.3
50TRF	0	50	50	64.1	58.1
Surrogate A	63	17	20	88	85
Surrogate B	69	17	14	87	85

4.1 Boundary conditions

The important boundary conditions are presented in Table D. The initial mixture properties were imposed at 99 CAD bTDC pressure, the initial pressure was extracted from the experimental pressure-crank angle profile. The initial EGR percentage by mass was assumed to be 5% or 7.5% depending on whether the mixture was pressure charged prior to induction or not respectively. The EGR composition was based on the species concentrations obtained from the previous cycle. Piston blowby parameters were determined by calibrating the pressure profile during compression and expansion such that a sufficient agreement was achieved with the experimental in-cylinder pressure-crank angle profile. The wall temperature was set at 410 K, the number of stochastic particles was 100 and a constant characteristic turbulent mixing time of 5 ms was adopted, throughout all the simulations.

Autoignition simulations are highly sensitive to the initial temperature imposed at the boundary condition (in this case at -99 CAD bTDC). Instantaneous measurements of this temperature were not available from experiments and when considering the influence of heat transfer, hot exhaust gas concentrations etc. can only be considered to be known to within a +/- 20 K range.

This study was an examination of the performance of the fuel mechanism and SRM code in the closed part of the cycle. In an attempt to reduce the uncertainty associated with computing the boundary condition, the initial temperature was set within a reasonable initial temperature range and then fine tuned to within the 20K for the 94 PRF blend at each Operating Point.

Hence, at each Operating Point the initial temperature was set as constant for all the adopted fuels.

Table D: Model boundary conditions

	Trapped EGR % vol	T (K) 99 CAD bTDC	P (bar) 99 CAD bTDC
OP1	5.0	400	3.84
OP2	5.0	425	3.84
OP3	7.5	430	1.7
OP4	7.5	430	1.7
OP5	7.5	499	1.6
OP6	7.5	499	1.5
OP7	5.0	421	3.25

4.2 Toluene Reference Fuel

A fuel model based on toluene/ n-heptane/ iso-octane chemistry was employed based on 137 species [7]. The mechanism was previously 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.

5. Results and discussion

5.1 HRM vs. SRM

Presented in Fig. 2 are the pressure-crank angle histories of the experiment, a Homogenous Reactor Method (HRM) case without blowby and an SRM case with blowby.

The HRM without blowby was adopted as representative of a typical approach to modelling HCCI engine combustion. The adoption of 100 particles for the SRM simulation was based on the convergence studies published previously [15].

The onset of ignition at 13 CAD bTDC of both computational approaches proved earlier than that observed in the experiment, however the pressure profile of the SRM was much improved over the HRM as compared to the experiment. This occurred most notably at 5 CAD bTDC, where the pressure departed significantly compared to the experiment and SRM case. Ignition occurred simultaneously in the HRM, whereas at this point, the particles in the SRM case were exposed to heat loss to the wall and the temperature was stratified leading to a slower heat release rate. Such differences are critical when estimating emissions, particularly NO_x and uHCs, as in the HRM case combustion ultimately occurred at temperatures in excess of the experiment and was too complete respectively.

5.2 Pressure profiles for individual operating points

The pressure-crank angle data obtained from simulating various fuels (where experimental pressure-crank angle data were available) at Operating Points (OPs) 1, 3, 4, 5, 6 and 7 is presented in Fig. 3. In all cases, the pressure due to compression and expansion prior and well after ignition are sufficiently within expected experimental uncertainties.

Generally in all cases, ignition and subsequent heat release were predicted with sufficient reliability, most notably at OP3, OP6 and OP7. At Operating Points 1 and 4, ignition onset times were predicted sufficiently, however subsequent heat release proved slightly too fast and two slow respectively. In both cases, it would have been possible to re-optimise the mixing and/or the heat transfer properties of the simulation for improved model performance. However, it was felt that "continual" re-optimisation would not be appropriate as the authors wished to remain as "predictive" in the methodology as possible.

At Operating Point 5, the heat release of the 64 TRF proved significantly slower than would be expected based on the performance of other similar blends at other Operating Points.

Overall, the SRM and TRF mechanism successfully predicted ignition onset and heat release with a high degree of accuracy for all blends including the three component Surrogates A and B.

5.3 PRF surrogate vs. TRF surrogate

Since experimental data in terms of pressure-crank angle was not always available, a summary of data in terms of the crank angle of 50% Heat Release (50%HR) for various fuels obtained at Operating Points 2 and 4 are presented in Table E.

In order to fully examine the "added value" of a TRF over a PRF mechanism, each experimental TRF blend was simulated using two methods (1) as a conventional TRF and (2) as a PRF surrogate selected on the basis of the equivalent RON.

At Operating Point 1 presented in Table E (a), overall the performance of the TRF surrogate proved adequate in successfully predicting 50%HR to within 2.5 CA. Conversely the PRF surrogate performed poorly for those mixtures with fuel "sensitivity". This was to be expected as this Operating Point was far removed from the RON and MON Operating Points and could be expected to have a *negative K*, see Fig. 1. Modern turbocharged gasoline engines with intercooling are anticipated to exhibit such *negative K* values.

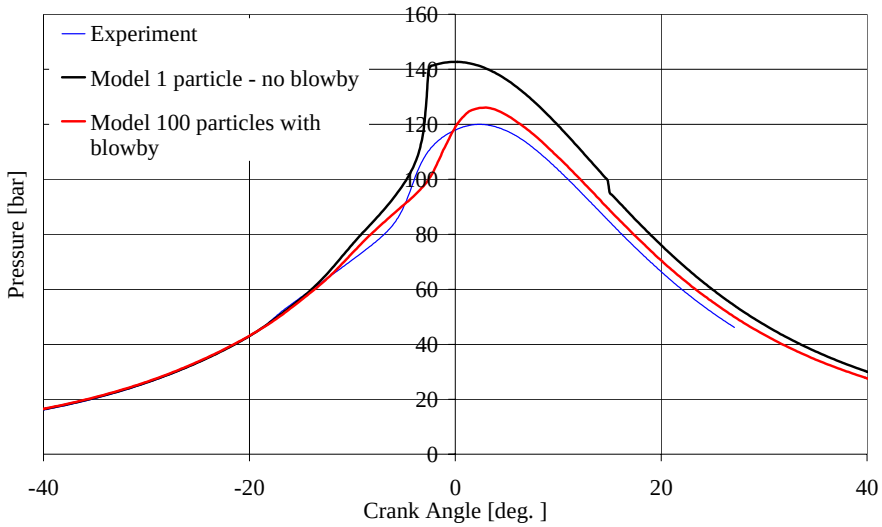
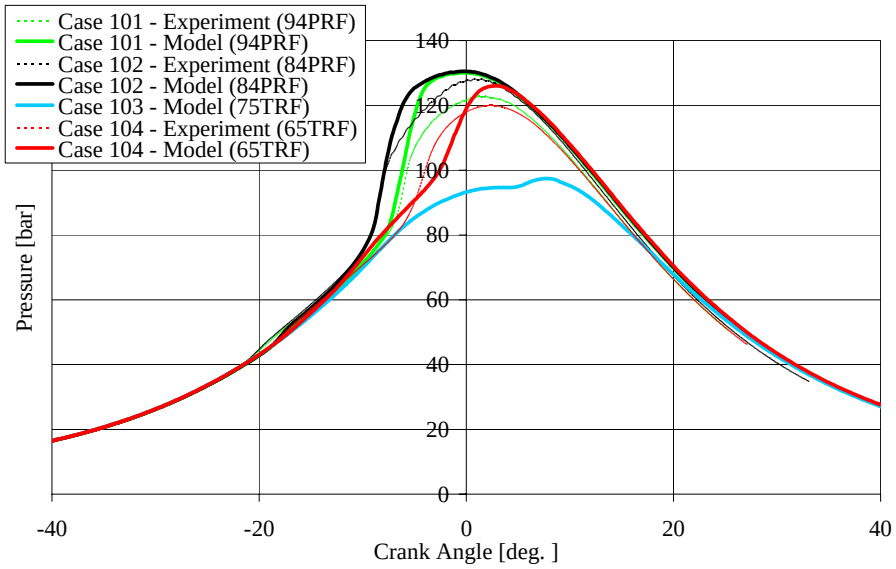
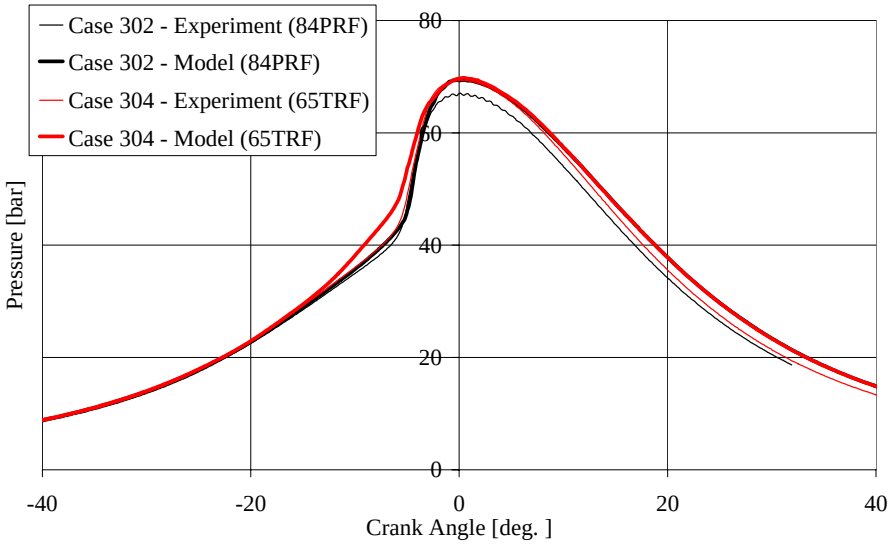


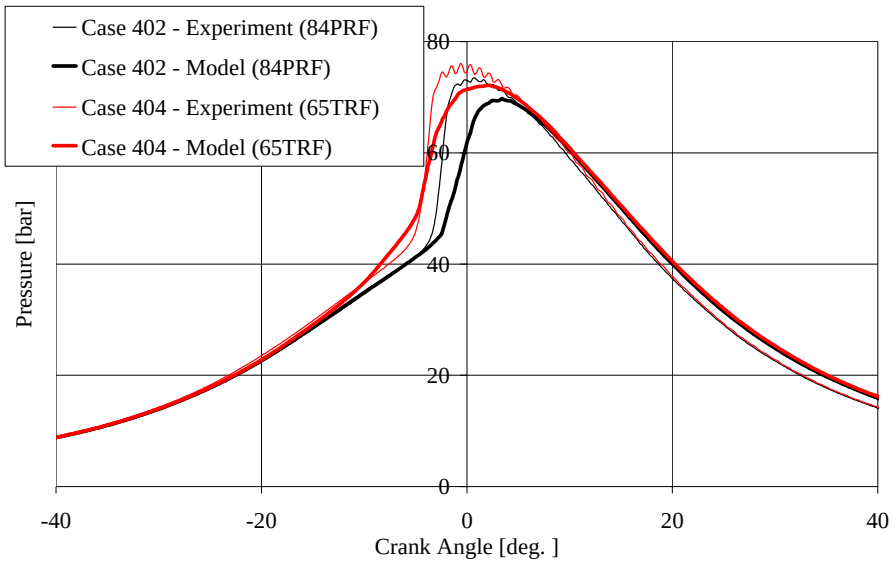
Fig. 2: Pressure vs. crank angle for a HRM (1 particle) and SRM (with 100 particles) based simulation



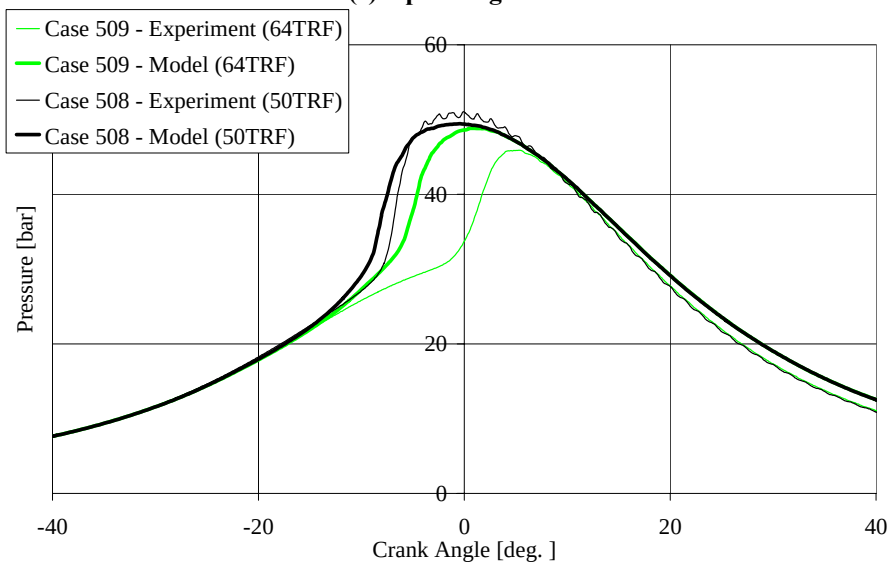
(a) Operating Point 1



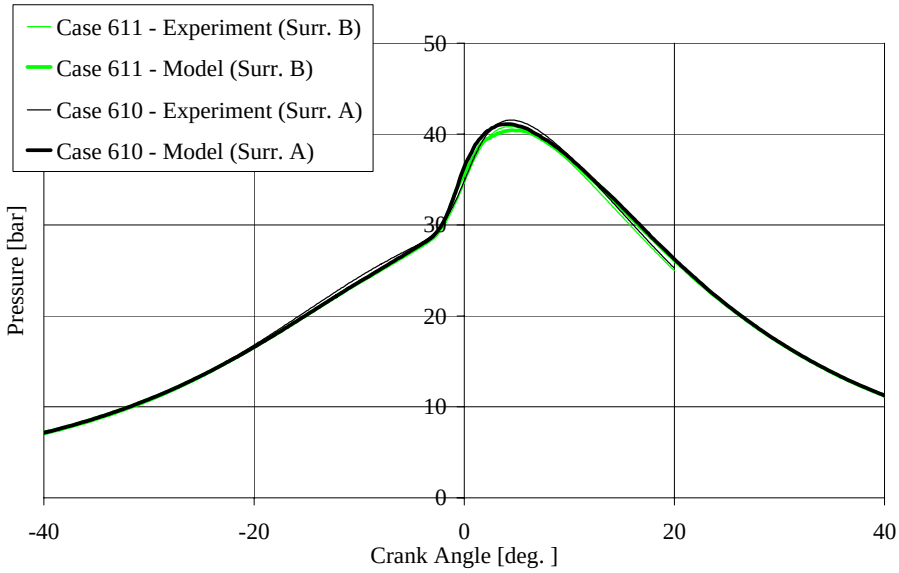
(b) Operating Point 3



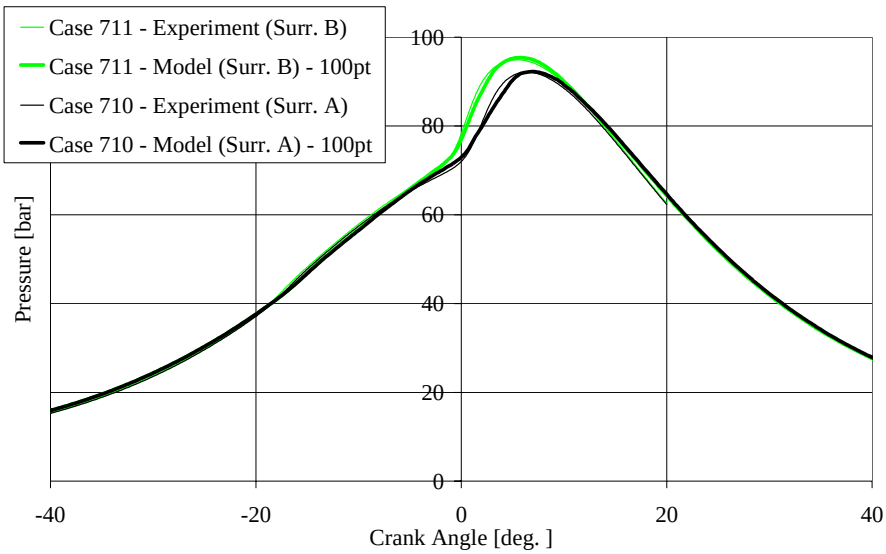
(c) Operating Point 4



(d) Operating Point 5



(e) Operating Point 6



(f) Operation Point 7

Fig. 3: Pressure vs. crank angle for experiment and model

This was most notable for the 75 TRF mixture, which in addition is also presented in terms of pressure-crank angle in Fig. 3(a). In this case, during experiments, no heat release rate was observed as the mixture would not ignite. The TRF surrogate case simulation predicted a very subtle heat release, indicating a condition close to misfire. Indeed if the simulation were fully coupled with a full intake and exhaust breathing routine, it would be expected that the imposed initial temperature of 425K and trapped EGR concentration of 5% may well be further reduced due to the observed low heat release from the previous cycle. This would consequently result in the total misfire reported experimentally. However if simulated using a PRF surrogate, the observation that the fuel was close to misfire would not have been observed. Indeed if the 94 PRF presented in Fig. 3(a) is assumed to be similar to the surrogate employed, regular HCCI combustion would be expected.

At Operating Point 4, presented in Table E(b) less notable differences are reported between the two surrogate mixtures. Based on Fig. 1, Operating Point 4, is closer to the RON and MON operating points, this suggests that in this range, differences between the two approaches are not so evident, that is a TRF is more similar to its equivalent PRF. This may well indicate why the PRF surrogate approach has proven (at least in part) effective in many solutions to date.

5.4 High load operating limit

The operating window of an HCCI engine is a major area of interest in developing the technology into a low emissions, high fuel economy and practical combustion mode. The high load operating point is of particular interest as the operating mode is limited by 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 [11].

Table E: Comparison of the model performance based on two assumptions (1) conventional TRF mechanism (2) a PRF surrogate

(a) Operating Point 1

	CAD at 50% Heat Release		
Fuel	Experiment	PRF Surrogate simulation	TRF Surrogate simulation
94 PRF	-5.6	-6.2	-
84 PRF	-8.0	-8.13	-
75 TRF	No ignition	-6.28	5.95
65 TRF	-3.5	-8.1	-1.71
62 TRF	-4.6	-8.64	-3.19

(b) Operating Point 4

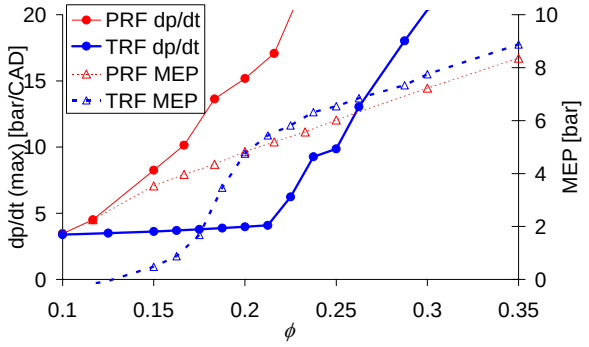
	CAD at 50% Heat Release		
Fuel	Experiment	PRF Surrogate simulation	TRF Surrogate simulation
94 PRF	8.0	6.37	-
84 PRF	-2.4	-5.41	-
75 TRF	7.3	6.52	0.2
65 TRF	-4.0	-1.18	-3.77
62 TRF	-5.4	-2.1	-4.78

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 considered representative of an engine operating point with *negative* and *positive K* respectively. In each case,

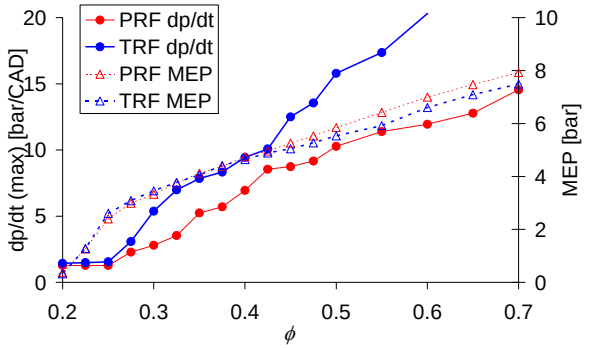
the parameters set out in Table D were employed but to simulate increasing load, the fuel concentration was increased. A 94 PRF and a 75 TRF (94.2 RON 82.6 MON) fuels were employed as they could be adopted as surrogates for gasoline.

Presented in Fig. 4 are the resulting MEP and $dp/dCAD_{(max)}$ for Operating Point 2 and 4. The value of $dp/dCAD_{(max)}$ was adopted as representative of the onset of HCCI engine "knock", whilst a definition of this value appears to be engine dependent [16, 17], it is considered to be of the order of 10 bar/CAD. Hence, in the case of Operating Point 2, by considering fuel "sensitivity", the Operating Window was shifted richer by 0.1 of an equivalence ratio and safely operated at a 40% greater load without knocking. Conversely at Operating Point 4, with a *positive K* value a fuel with sensitivity proved less resistant to autoignition and only lower loads than the equivalent PRF were achieved. Similar trends were observed for other combustion characteristics such as CAD at 50% heat release.

It is important to note that the amount of EGR was not varied in this exercise and may well be employed successfully to further extend the operating window.



(a) Operating Point 2



(b) Operating Point 4

Fig. 4 MEP and $dp/dCAD_{(max)}$ against equivalence ratio for two Operating Points

The use of PRF or TRF blends in this study have highlighted a shortcoming in the previous methodology of predicting autoignition in engines with fuels with "sensitivity". Previous attempts of examining these types of fuels have not properly captured the chemistry associated with a full range of Operating Points and in particular those furthest removed from the RON/MON test operating points.

This work has demonstrated that a PRF mechanisms can be successfully optimised against a fuel with "sensitivity" at a single operating point, however once employed at another condition the reliability is reduced. Hence, by employing the TRF mechanism, there is less need and justification to continually re-optimise and correlate autoignition models for engine applications.

Whilst simulations were carried out at a fixed trapped EGR concentration, they demonstrated the HCCI engine window could well be extended to higher loads if Operating Points with a *negative K* were employed and mixtures with a "greater" fuel sensitivity adopted. Indeed further optimisation in terms of EGR may well yield increased engine loads below the "knock" limit.

6. Conclusions

A chemical kinetic mechanism for toluene-reference-fuels has been implemented into the SRM to examine HCCI engine combustion for a variety of fuels and operating conditions.

The SRM approach proved more consistent with the experiments in terms of heat release profiles compared to the equivalent HRM approach. The SRM and TRF mechanism were successfully validated against a range of experimental data with a high degree of accuracy.

Results indicated significantly improved performance for examining fuels with fuel sensitivity and highlighted the need for considering these aspects in a range of operating conditions and understanding the HCCI operating window.

Acknowledgements:
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