

# Simulating the Octane Appetite of SI Engines: The Influence of Chemical Mechanisms

Kieran P. Somers<sup>\*1,2</sup>, Roger F. Cracknell<sup>2</sup>, Henry J. Curran<sup>2</sup>

<sup>1</sup>Combustion Chemistry Centre, National University of Ireland, Galway, Ireland

<sup>2</sup>Shell Global Solutions, UK

## Abstract

The RON and MON standards of fuel anti-knock quality are no longer a *de facto* benchmark of fuel knock-resistance, owing to the diverging operating conditions of CFR engines and modern downsized boosted engines, and the fundamentally different chemical kinetic behaviour of primary reference fuels and real gasoline fuels. The octane index, OI, may provide a more practically relevant measure of fuel anti-knock quality by linear extrapolation of the RON and MON numbers *via* an engine-operating-condition-dependent factor, K:

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

where the term in parenthesis is defined as the fuel sensitivity, S.

Here, a previously developed method to simulate the octane index of SI engines is used to investigate the influence of detailed chemical mechanisms on the predicted anti-knock quality of gasoline surrogate fuels. Through simulations of ignition delay times of these mixtures “in-engine” *via* 0-D homogeneous constant-volume reactors, we highlight a significant variation in ignition delay predictions for a small sample of gasoline surrogate mechanisms. The results, although preliminary, highlight the need for a) a more rigorous benchmarking of any proposed gasoline surrogate mechanisms from the literature and b) the development of an industrially applicable mechanism based on the state-of-the-art derived from a).

## Introduction

Since the development of the spark-ignition internal combustion engine, autoignition induced engine knock has been a constraining phenomenon in terms of engine performance and efficiency. Finite reserves of fossil fuels, increasingly stringent regulations governing minimum fuel specifications, and maximum vehicle emissions, are driving the synergistic development of knock-resistant gasoline fuels to act as energy carriers in modern and future SI engines.

Historically, the anti-knock quality of a fuel has been defined via its Research Octane and Motor Octane Numbers (RON and MON), which are inextricably linked to the autoignition properties of *i*-octane/*n*-heptane primary reference fuel (PRF) mixtures in Co-operative Fuels Research (CFR) engines.

It is now well-known that RON and MON alone do not adequately describe the anti-knock quality of a practical fuel over the complete range of operating conditions of modern downsized and boosted engines [1, 2]. Two likely reasons exist for this divergence: (a) the operating conditions in CFR engines are not representative of those in modern SI engines, and (b) unlike PRF fuels, whose RON = MON, real fuels exhibit sensitivity, S, defined as the difference in the RON and MON.

As a result, in 2001 Kalghatgi [1, 2] proposed a more appropriate measure of anti-knock quality of a fuel, known as the Octane Index (OI), which is a linear function of RON and MON,  $OI = RON - KS$ .

K, or the K-value, is an extrapolation factor for RON and MON which is dependent on the operating conditions of the engine, that is, the temperature and pressure history during the course of each cycle. At the time, Kalghatgi [1, 2] showed that K tended to assume a

negative or only slightly positive value for a range of European and Japanese cars operating on various fuels. The significance of the result is that fuels with a high sensitivity (i.e. a *lower* MON) tend to have a greater anti-knock quality in modern SI engines where, for a given pressure, in-cylinder temperatures tend to be lower than those found in the RON and MON tests [1, 2]. Studies by Mittal and Heywood [3] and others [4, 5], reinforce the findings of Kalghatgi [1, 2].

Indeed, Kalghatgi and co-workers [6] recently proposed a new scale with which to define the anti-knock quality of practical gasoline fuels—the Toluene Number (TN) scale. Whether this scale is adopted across the combustion community remains on open question, but it is abundantly clear that one cannot garner a complete understanding of the anti-knock quality of a fuel based on the RON and MON values alone.

With the K-value method having gained some credence since being proposed by Kalghatgi, Davies *et al.* [7] endeavoured to develop a method to simulate the OI, and thus K-value, of an SI engine through 0-D chemical kinetic simulations of ignition delay times. Their work, to be described in more detail below, forms an important foundation for *this study*.

From a chemical kinetics perspective, the combustion chemistry of PRFs has been studied comprehensively over the last 4–5 decades. The literature is too expansive to venture into any great detail herein, although a recent review of gasoline and diesel surrogate fuel modelling from Battin-Leclerc [8] should provide the reader with an overview of the research area. The work of Curran and co-workers [9, 10] should provide the reader with an expert overview on the combustion chemistry of PRF fuel oxidation,

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\* Corresponding author: [Kieran.Somers@nuigalway.ie](mailto:Kieran.Somers@nuigalway.ie)  
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with a recent review of low-temperature oxidation by Zádor *et al.* perhaps also of interest [11].

Despite the large efforts focusing on improving our understanding of hydrocarbon combustion, no unambiguous description of the combustion of PRFs or toluene reference fuels (TRFs) exists in the literature. This is primarily the result of the divergent development of kinetic mechanisms over the years—rate constant rules applied to PRF oxidation can vary in their origin, as can the provenance of the C<sub>0</sub>-C<sub>4</sub> base mechanisms which form the foundation of our understanding of the combustion of larger practical fuels. This is coupled with the fact that different kinetic mechanisms tend to be validated in different experimental regimes of  $T$ ,  $p$  and  $\Phi$ , and the complex composition of “real” gasoline fuels leads to problems in formulating surrogates which can replicate the physicochemical and combustion properties of real fuels.

Many of these problems have been alluded to by Simmie [12] in 2003, but modelling these complex systems is no menial task, and it appears that we are still some way away from reaching a unified quantitative, qualitative and predictive understanding of gasoline and diesel fuel combustion. Ultimately, from both an industrial and academic perspective, there is no single mechanism which can be described as the *de facto* state-of-the-art with respect to the modelling of gasoline fuel combustion, possibly owing to a lack of benchmarking of available mechanisms in the literature.

*This study* utilises the methodology of Davies [7] to simulate the OI of an SI engine under a single engine condition, but with various chemical mechanisms. The aim is to assess how dependent the computed OI and K-values are on the chemical kinetic mechanism employed in the simulation, and thus, to guide the choice of kinetic mechanism employed for this industrial application in the future.

## Methodology

The method developed by Davies is described in detail elsewhere [7], but briefly re-iterated, one must have information concerning:

- In-cylinder pressure versus crank-angle degree (CAD) (derived from a knocking engine experiment)
- In-cylinder volume versus CAD derived from the known engine geometry (optional)
- In-cylinder temperature versus CAD, derived from the above, or from an appropriate engine simulation
- Equivalence ratio ( $\Phi$ )
- Spark-timing
- Mass of cylinder contents (including residual gas)
- Engine speed (RPM)

0-D constant-volume simulations are then carried out under the known conditions of  $p$ ,  $T$ ,  $V$  and  $\Phi$  at each CAD, and the ignition delay time,  $\tau$ , is computed. The Livengood-Wu integral [13] is then applied to calculate

Vol %		Octane Properties		
Toluene	n-Heptane	RON	MON	S
74	26	92.85	78.65	14.20
73	27	91.84	77.72	14.13
71	29	89.82	75.85	13.97
70	30	88.80	74.91	13.89
69	31	87.77	73.96	13.81
68	32	86.73	73.01	13.72

Table 1: Details of surrogate mixtures used to represent gasoline fuels as part of this modelling study.

Engine Speed / rev min <sup>-1</sup>	2000
$\Phi$	1.00
Spark Timing / CAD bTDC	2.5
$p$ / bar	1.23–133.1
$T$ / K	250–802
Residual Mass Fractions	
N <sub>2</sub>	7.639×10 <sup>-1</sup>
O <sub>2</sub>	2.192×10 <sup>-1</sup>
CO <sub>2</sub>	1.101×10 <sup>-2</sup>
H <sub>2</sub> O	5.286×10 <sup>-3</sup>
CO	5.891×10 <sup>-4</sup>
H <sub>2</sub> O	1.877×10 <sup>-5</sup>

Table 2: Experimental conditions used in simulation (bTDC = before top dead centre).

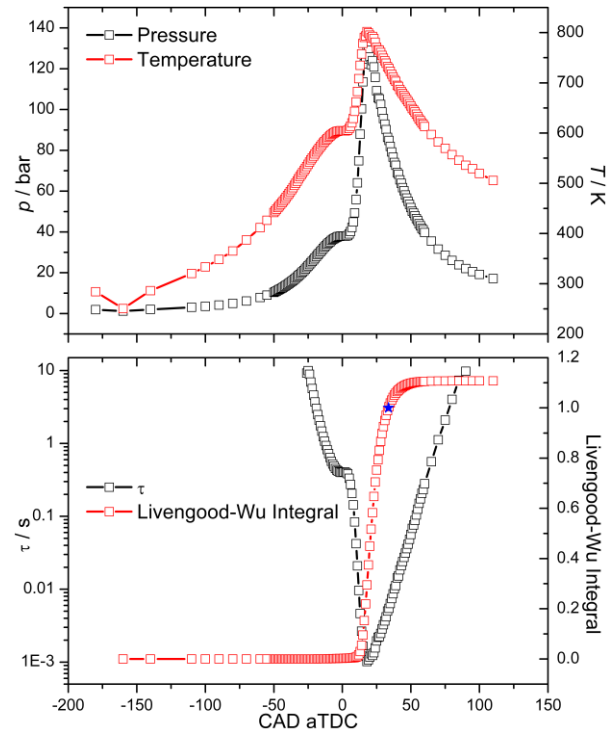


Figure 1: (a) In-cylinder pressure and temperature profiles from Remmert *et al.* [5] and (b) ignition delay times and Livengood-Wu integral computed based on the  $p$ - $T$  profiles from (a). Simulations were carried out using the Andrae [14] mechanism for a  $\Phi = 1.00$  *i*-octane/air (PRF 100) mixture with residuals gases as reported in Table 2. The blue star indicates where the Livengood-Wu integral = 1 (CAD<sub>auto</sub>).

the CAD at which knock onset is observed, CAD<sub>auto</sub>, with Figure 1 illustrating the concept. CAD<sub>auto</sub> is first computed for a range of *n*-heptane/*i*-octane mixtures

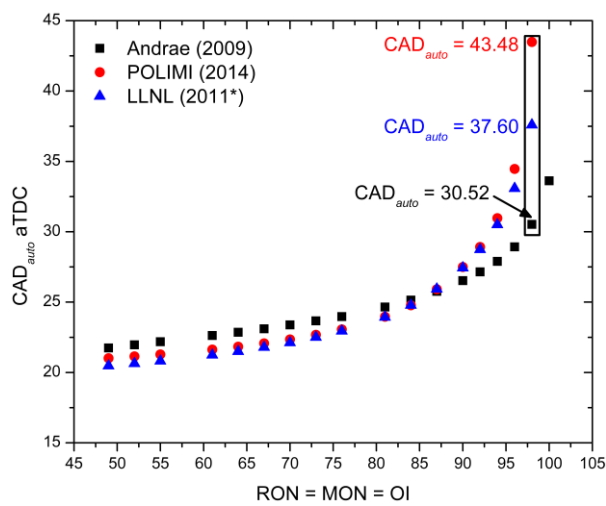


Figure 2: Computed crank-angle degree of autoignition ( $CAD_{auto}$ ) vs octane index (OI) for *n*-heptane/*i*-octane PRFs.  $CAD_{auto}$  are specifically reported for the PRF 98 fuel simulations enclosed by the black box.

with varying octane numbers, and thus OI, in order to construct a PRF calibration curve (OI vs  $CAD_{auto}$ ). 5<sup>th</sup>-order polynomials have been used to correlate OI with  $CAD_{auto}$  in *this work*. Note that by definition,  $RON = MON = OI$  for these PRF mixtures. A range of surrogates with different RON and MON, i.e. fuel sensitivity, are then simulated and the  $CAD_{auto}$  derived. The computed  $CAD_{auto}$  for each surrogate is then used in conjunction with the PRF calibration curve to derive its OI, which once known, can be used to compute  $K$  via  $K = (RON - OI) \times (RON - MON)^{-1}$ .

19 PRF mixtures with OI ranging from 100 to 49 have been used to construct OI calibration curves, with 6 gasoline surrogates also simulated, Table 1. Three chemical kinetic mechanisms have been applied to assess their influence on the computed  $K$ -values. The first is the Andrae and Head [14] semi-detailed gasoline surrogate mechanism (143 species, 672 reactions) which has historically [5, 7] been used at Shell to interpret and model engine experiments. The second is a very recently validated reduced gasoline surrogate mechanism (157 species, 3465 reactions) from Ranzi *et al.* [15], POLIMI mechanism henceforth, and the third is a reduced version [16] (679 species, 3479 reactions) of the detailed Lawrence Livermore National Lab (LLNL) gasoline surrogate mechanism from 2011 [17].

The required experimental input data, primarily the knocking pressure trace and accompanying temperature profile, have been taken from the work of Remmert *et al.* [5] with relevant details summarised in Table 2.

All simulations have been carried out with the Aurora module of Chemkin-PRO [18] (constant volume batch reactor) with the ignition delay time defined as the time at which the temperature has risen by 400 K from its initial value.

The maximum simulation time was set to 10 s as at longer ignition delay times, the contribution to the Livengood-Wu integral is minimal, Figure 1.

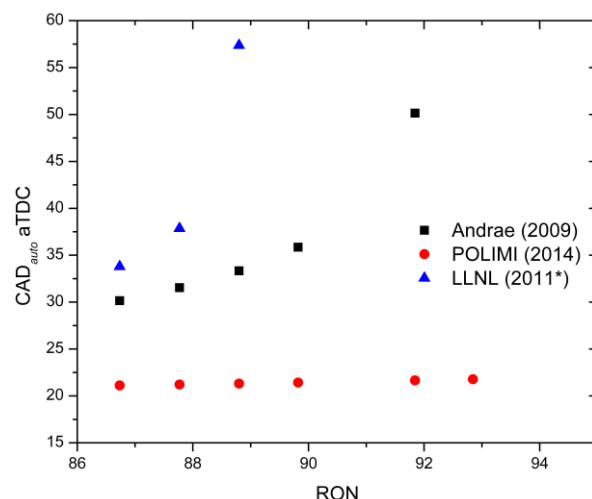


Figure 3: Computed crank-angle degree of autoignition ( $CAD_{auto}$ ) vs RON for the *n*-heptane/toluene surrogates defined in Table 1. The absence of data for a given RON fuel indicates that the Livengood-Wu integral did not reach unity.

## Results and Discussion

For the engine experiment being analysed, the three chemical kinetic mechanisms employed will be compared on three fronts, 1)  $CAD_{auto}$  for the PRF calibration curves, 2)  $CAD_{auto}$  for the 6 *n*-heptane/toluene surrogate mixtures, and ultimately, 3) the computed OI and  $K$ -values for each mixture.

Calibration curves are shown in Figure 2 for the 19 PRF mixtures simulated using the three different chemical mechanisms. If no symbol is present for a given mixture then either the computed  $CAD_{auto}$  was greater than 45 degrees after top dead centre (aTDC) or the Livengood-Wu integral never equated to 1, thus indicating that knock would not occur under these engine conditions.

Below OI = 84, the three mechanisms show reasonably similar qualitative and quantitative behaviour— $CAD_{auto}$  varies by only  $1.14 \pm 0.62$  CADs and slopes are of a similar order. However, for PRFs with octane number greater than this, the three mechanisms start to diverge in their predictions. The Andrae mechanism notably crosses-over the other two mechanisms as the fuel approaches 100% [*i*-octane]. Although the POLIMI and LLNL mechanisms tend to follow a similar qualitative trend, there are still large quantitative differences in the computed  $CAD_{auto}$ . For example, for PRF 100 fuel, the reduced LLNL mechanism predicts  $CAD_{auto} = 60.07$  degrees, the Andrae mechanism predicts  $CAD_{auto} = 33.62$  degrees, and POLIMI mechanism predicts that knock will *not* occur. The results for PRF 98 fuel, highlighted in Figure 2, illustrate a similar trend, with a  $\approx 13^\circ$  spread in the computed  $CAD_{auto}$ . The largest differences in the predictions are therefore in the region of octane number phase-space of relevance to many practical gasoline fuels (RON and MON > 85), which is a somewhat concerning result.

Figure 3 similarly compares the computed  $CAD_{auto}$  vs RON for the surrogates defined in Table 1. There is

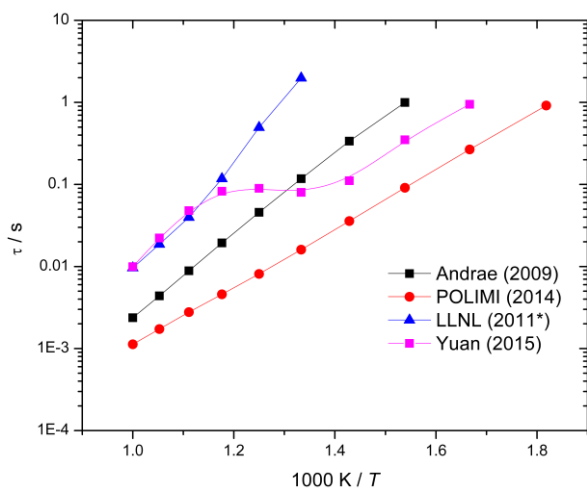


Figure 4: Ignition delay time ( $\tau$ ) simulations of stoichiometric toluene/air mixtures at 20 atm with various chemical mechanisms.

clearly a significant disagreement amongst the three chemical mechanisms with respect to the reactivity of these *n*-heptane/toluene mixtures. Given that a large percentage of these surrogate fuels are composed of toluene (minimum 68 vol. %), and that the computed  $CAD_{auto}$  diverges as the proportion of toluene in the mixture increases, one must conclude that the differences in the computed  $CAD_{auto}$  derive from differences in the chemical kinetics and thermodynamics employed in the three mechanisms to describe the low-to-intermediate-temperature oxidation of toluene.

POLIMI mechanism would imply that under these engine conditions,  $CAD_{auto}$  is independent of toluene concentration, and thus RON—a counter-intuitive trend which is not supported by the other mechanisms. Conversely, the reduced LLNL mechanism predicts that above a 70 volume % of toluene in the fuel, the mixture becomes so knock resistant that autoignition does not occur. The mechanism of Andrae predicts  $CAD_{auto}$  somewhere between these extremes of reactivity. These findings are supported by 0-D batch reactor simulations of the ignition of stoichiometric toluene/air mixtures at a somewhat arbitrary representative pressure of 20 atmospheres, Figure 4, where the order of reactivity  $POLIMI > Andrae > LLNL$  is observed.

Note that Yuan *et al.* [19, 20] recently carried out an extensive re-validation of the combustion kinetics of toluene, validating their model against oxidation and pyrolysis speciation data in flow- and jet-stirred reactors, ignition delay time data in shock tubes, and laminar flame speciation and flame speed measurements, over wide ranges of temperature, pressure and equivalence ratio. However, no validation was carried out against ignition delay times at temperatures below 920 K possibly owing to a lack of available experimental data. If their [19, 20] chemical mechanism is used to simulate toluene ignition under conditions in Figure 4, a negative temperature coefficient (NTC) regime is observed from 750–850 K.

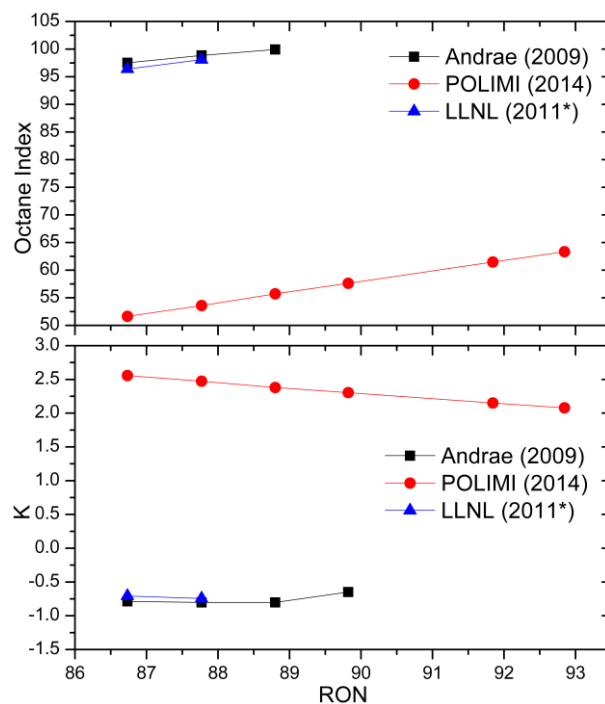


Figure 5: Computed octane indices (OI) and K-values vs RON for gasoline surrogates described in Table 1. If no data are presented for a given model, it is due to the computed OI being outside the range of the calibration curve, i.e.  $OI > 100$ .

This NTC regime is not to be expected, as the typical [9–11]  $R+O_2 \leftrightarrow RO_2 \leftrightarrow QOOH \leftrightarrow \text{product(s)}$  pathways which typify this behavior are inhibited in the benzyl+ $O_2$  system owing to a very shallow well-depth for the  $RO_2$  radical [21]. Similarly, NTC behavior is not observed in the oxidation of propene owing to the dominant fuel radical formed from H-atom abstraction reactions being allylic in nature [22].

With toluene being an important component of any gasoline surrogate fuel, the results highlight the need to more closely consider its low-to-intermediate temperature oxidation in the future.

Now we consider the octane indices and K-values computed for the gasoline surrogates based on their computed  $CAD_{auto}$  (Figure 3) and the PRF calibration curves show in Figure 2.

The first point of note is the large discrepancy between the predictions of the POLIMI mechanism, and the Andrae and LLNL mechanisms, the latter two being in quite good agreement with each other with respect to the computed OI and K-values, Figure 5. Also, the latter two mechanisms more closely emulate the experimental trend that K assumes a negative value in modern SI engines [1–5], with the positive K-values predicted by the POLIMI mechanism contrasting with recent experimental findings [1–5].

These results raise some interesting topics for discussion, such as why do the LLNL and Andrae mechanisms agree so closely with respect to their computed OIs and K-values, despite the fact that there is a large difference in the computed  $CAD_{auto}$  for both the PRF mixtures used to construct their calibration curves, and the toluene/*n*-heptane gasoline surrogate mixtures.

This finding is likely the result of some error-cancellation effects within the mechanisms—the LLNL predicts slower  $CAD_{auto}$  for both the PRF and toluene/*n*-heptane mixtures when compared with the Andrae mechanism. So despite the large differences in the absolute  $CAD_{auto}$  values computed by these two mechanisms, by arriving at similar relative reactivities for the PRF and toluene/*n*-heptane surrogate mixtures, similar K-values are derived.

The calibration curves for POLIMI and LLNL mechanisms were in reasonable qualitative and quantitative agreement, but the drastically different reactivities predicted by these mechanisms for the toluene/*n*-heptane surrogates manifests as large differences in the computed OIs and K-values under these engine conditions.

## Conclusions

Engine knock remains one of the key constraints with respect to the efficiency and performance of SI engines. With the design and operating conditions of modern SI engines having diverged greatly from the CFR engines which were used to originally define the RON and MON scales, the need for extrapolative models for these two ubiquitous measures of fuel anti-knock quality are required, such as the K-value and Toluene Number (TN) scales suggested by Kalghatgi and co-workers [1, 2, 6]

*This work* used the computational method of Davies *et al.* [7] to derive K-values for a range of gasoline surrogate fuels under a single engine operating condition [5], but with three unique chemical kinetic mechanisms [14–17].

The crank-angle degree of autoignition ( $CAD_{auto}$ ) of a range of *n*-heptane/*i*-octane PRF fuels was determined in order to construct PRF calibration curves that could be used to compute the octane index (OI), and thus K-value, for six gasoline surrogates. The calibration curves constructed from the three chemical kinetic mechanisms were in reasonable agreement for PRF fuels with OI in the range 49–90. At higher concentrations of *i*-octane (RON 90 → 100), the three mechanisms start to diverge in their predictions of  $CAD_{auto}$ , with an approximately 13° variation observed for PRF 98 across the three mechanisms.

All three mechanisms also differ substantially with respect to the  $CAD_{auto}$  computed for a range of gasoline surrogates with RON and MON varying from 86.73–92.85 and 73.01–78.65 respectively. Despite this, the Andrae [14] and LLNL [16, 17] mechanisms derive similar K-values for the surrogate fuels, as these mechanisms tend to predict similar *relative* reactivities for the PRF fuels and the toluene/*n*-heptane surrogate fuels. The mechanism of Ranzi *et al.* [15] (POLIMI mechanism), despite showing similar  $CAD_{auto}$  to LLNL mechanism for the PRF fuels, arrives at very different K-values upon simulation of knock-onset for the toluene/*n*-heptane surrogate fuels. The reason for the different K-values arrived at by the POLIMI mechanism [15] and those of the Andrae [14] and LLNL [16, 17]

mechanisms, is shown to likely derive from differences in the sub-mechanisms used to describe the oxidation of toluene. A recently validated mechanism for toluene oxidation [19, 20] is also compared with the three mechanisms used as part of *this work* for the ignition of stoichiometric toluene/air mixtures at 20 atm from temperatures of 600–1000 K. The results highlight wide variations in the predicted ignition delay times for these toluene mixtures across the four mechanisms employed, with one of the mechanisms showing a pronounced NTC region under these conditions—a counter-intuitive result as one would not anticipate toluene to exhibit the archetypal low-temperature reaction pathways which lead to NTC behaviour in PRF fuel combustion.

Ultimately, given that toluene should form a major component of any gasoline surrogate fuel, the results may highlight the need to further investigate its oxidation in this temperature range, as the majority of data used to re-validate the chemical mechanism for toluene oxidation [19, 20] were obtained at temperatures greater than 900 K.

Based on the preliminary results presented herein, one must conclude that several recently proposed gasoline surrogate mechanisms show quantitatively different chemical kinetic behaviour when used to model the current experiments. Moving forward, there may be a need to re-evaluate the combustion of both the PRFs, and toluene, in order to arrive at a modern gasoline surrogate mechanism whose thermochemical and kinetic data have been validated against a wide-range of fundamental laboratory and in-engine experiments. Not only this, but it would be desirable that any future validation studies for gasoline surrogate fuels incorporate a benchmarking aspect to the work, in order to advise on the current state-of-the-art in gasoline surrogate mechanisms in the chemical literature.

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