

Provided by the author(s) and NUI Galway in accordance with publisher policies. Please cite the published version when available.

Title	A chemical kinetic interpretation of the octane appetite of modern gasoline engines
Author(s)	Somers, Kieran P.; Cracknell, Roger F.; Curran, Henry J.
Publication Date	2018-06-29
Publication Information	Somers, Kieran P., Cracknell, Roger F., & Curran, Henry J. (2019). A chemical kinetic interpretation of the octane appetite of modern gasoline engines. <i>Proceedings of the Combustion Institute</i> , 37(4), 4857-4864. doi: <a href="https://doi.org/10.1016/j.proci.2018.05.123">https://doi.org/10.1016/j.proci.2018.05.123</a>
Publisher	Elsevier
Link to publisher's version	<a href="https://doi.org/10.1016/j.proci.2018.05.123">https://doi.org/10.1016/j.proci.2018.05.123</a>
Item record	<a href="http://hdl.handle.net/10379/15122">http://hdl.handle.net/10379/15122</a>
DOI	<a href="http://dx.doi.org/10.1016/j.proci.2018.05.123">http://dx.doi.org/10.1016/j.proci.2018.05.123</a>

Downloaded 2022-08-14T22:04:07Z

Some rights reserved. For more information, please see the item record link above.



# A Chemical Kinetic Interpretation of the Octane Appetite of Modern Gasoline Engines

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

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

<sup>b</sup>*Shell Global Solutions, UK*

---

## Abstract

Fuel anti-knock quality is a critical property with respect to the effective design of next-generation spark-ignition engines which aim to have increased efficiency, and lower emissions. Increasing evidence in the literature supports the fact that the current regulatory measures of fuel anti-knock quality, the research octane number (RON), and motor octane number (MON), are becoming decreasingly relevant to commercial engines. Extrapolation and interpolation of the RON/MON scales to the thermodynamic conditions of modern engines is potentially valuable for the synergistic design of fuels and engines with greater efficiency. The  $K$ -value approach, which linearly weights the RON/MON scales based on the thermodynamic history of an engine, offers a convenient experimental method to do so, although complementary theoretical interpretations of  $K$ -value measurements are lacking in the literature.

*This work* uses a phenomenological engine model with a detailed chemical kinetic model to predict and interpret known trends in the  $K$ -value

---

\*Corresponding author: Combustion Chemistry Centre, National University of Ireland, Galway, Ireland. Phone: +353-86-1250478. Email: Kieran.Somers@nuigalway.ie

with respect to engine intake temperature, pressure, and engine speed. The modelling results support experimental trends which show that the  $K$ -value increases with increasing intake temperature and engine speed, and decreases with increasing intake pressure. A chemical kinetic interpretation of trends in the  $K$ -value based on fundamental ignition behaviour is presented. The results show that combined experimental/theoretical approaches, which employ a knowledge of fundamental fuel data (gas phase kinetics, ignition delay times), can provide a reliable means to assess trends in the real-world performance of commercial fuels under the operating conditions of modern engines.

*Keywords:*

Gasoline, Spark-Ignition, Octane Number, Chemical Kinetics, Ignition Delay Time

---

## 1. Introduction

The development of novel fuel-engine technologies is being driven by increasingly stringent regulations [1], which aim to mitigate the effects of greenhouse gases and harmful emissions on the environment and on human health. For spark-ignition (SI) gasoline-fuelled engines there is currently a major trend towards the development of downsized and boosted engines. These technologies may enable efficiency improvements *via* reduced friction and pumping losses, whilst still retaining vehicular performance. Despite the reduction in parasitic losses achievable through improved engine design, the efficiency of such technologies will remain dependent on the chemical structure of the fuel being combusted.

Phenomonologically the basis for engine knock is well established [2], and

is generally attributed to the pressure oscillations which result from the auto-ignition of the unburnt gas charge as it is compressed by the piston and/or the propagating flame front, with the process controlled by both the engine and fuel design. Presently, the efficiency of a fuel in a SI engine is regulated *via* its octane number(s), namely, the Research Octane Number (RON) and Motor Octane Number (MON). Both of these properties are measured under specific operating conditions in Cooperative Fuels Research (CFR) engines, the design of which dates back to the 1930's. The ASTM methods to measure RON and MON in CFR engines are well-described elsewhere [3, 4], and historically these tests have served as simple and reliable metrics to determine and regulate the efficiency of complex fuels for use in the commercial fleet.

However, the relevance of the CFR-PRF approach to understanding more complex fuel-engine technology combinations is becoming increasingly questionable [5, 6, 7, 8] due to changes in the design of commercial fuels, and engine and vehicular hardware. It is well-known [9, 10, 11, 12] that PRF blends are not fully representative of the combustion chemistry of refinery-derived commercial fuels, which differ from PRFs as a result of their complex composition. This leads to differences in their fundamental combustion properties (e.g. ignition delay time, laminar flame speed) resulting in an octane sensitivity,  $S$ , which is defined as the difference in its measured RON and MON. As a result of this fuel sensitivity, the relative anti-knock quality of a commercial fuel versus a PRF blend will be dependent on the thermodynamic conditions of temperature and pressure experienced by the unburnt end-gas, which will vary depending on whether the engine is operating under the conditions of the RON test, the MON test, or as is more likely in modern

commercial vehicles, some other condition which is not equivalent to either of these tests [5, 6, 7, 8].

To reduce the need for laborious measurements of the efficiency of a given fuel in a given engine, cost-effective methods to map the RON and MON values to the conditions experienced in commercial engines would be of great use industrially and academically. One such method is the “ $K$ -value” approach offered by Kalghatgi [5, 6], which aims to address the difference between CFR and modern engines *via* a linear weighting factor,  $K$ , thus allowing the derivation of an Octane Index (OI):

$$\text{OI} = \text{RON} - K (\text{RON}-\text{MON}) \quad (1)$$

$K$  is experimentally determinable [5, 6, 7, 8, 13, 14, 15, 16, 18, 19, 20, 21, 22] and is solely dependent on the time-dependent temperature and pressure conditions experienced by the end-gas during a combusting cycle. In practical terms, a value of  $K = 0$  implies a RON-like thermodynamic history,  $K = 1$  indicates a MON-like thermodynamic history, and  $K = 0.5$  implies a thermodynamic history indicative of the anti-knock index (AKI) employed in the US as a measure of fuel-efficiency.

Numerous studies have determined  $K$ -values from engine and vehicular performance measurements [5, 6, 7, 8, 13, 14, 15, 16, 18, 19, 20, 21, 22]. These works show that  $K$ -values are negative for modern engines [5, 6, 8, 18, 19, 20, 21, 22], which tend to operate under thermodynamic conditions which are “beyond RON”—for a given in cylinder-pressure, the end-gas tends to be at a lower temperature than the RON test. From a fuel chemistry perspective, the significance of a negative  $K$ -value is that an efficiency benefit can be extracted

from a fuel by increasing its RON, or counter-intuitively, by *decreasing* its MON. These studies also show that  $K$ -values increase with increasing intake temperature [7, 13] and increasing RPM [5, 7, 13, 19], and decrease with increasing intake pressure [17, 18, 19, 21]

Whilst there are an increasing number of studies which have experimentally determined  $K$ , complementary kinetic modelling studies are virtually **non-existent** in the literature [14, 19]. An exploratory work from the present authors showed [23] that the computation of the OI and  $K$ -value can be sensitive to the chemical mechanism employed in the simulation method of Davies *et al.* [14]. **In particular, the approach was used to highlight order-of-magnitude variations in the predictions of toluene ignition delay times from chemical mechanisms available in the literature** [23, 24]. Given a lack of an extensive assessment of trends in  $K$ -value using the above approach [14], *this work* aims to rationalise experimentally observed trends in  $K$ -value over a broader range of conditions than previously studied [14, 23], and to interpret these trends in light of the underlying ignition behaviour.

## 2. Modelling Approach

The method to compute  $K$ -values [14] is computationally efficient and requires only basic data in the form of engine speed, intake temperature and a measured pressure history for the  $K$ -value to be computed [14, 19]. Knowing the heat capacity of the gas-phase fuel-air mixture, and assuming an adiabatic and isentropic compression-expansion process, one can derive an estimate of the end-gas temperature with crank angle degree. 0-D ignition delay times ( $\tau$ ) are then computed at each CAD, and the Livengood-Wu integral [25] is

applied to estimate the crank-angle degree of knock onset ( $CAD_{auto}$ ). This approach is carried out for a series of PRFs in order to construct a calibration curve of  $CAD_{auto}$  versus OI.  $CAD_{auto}$  is then computed for a fuel where  $RON \neq MON$  and  $S \neq 0$ , and its OI is then computed from the calibration curve *via* interpolation. Knowing the RON and MON of the sensitive fuel from experimental measurement, and with the computational estimate of the OI, the  $K$ -value can be determined by rearrangement of Equation 1. Examples of the simulation method are presented in the electronic supplementary information (ESI).

A consistent matrix of experimental engine data would provide an ideal test-set to evaluate the rigour and utility of the approach of Davies *et al* [14]. However, in the absence of such data, we require only engine-like data to rationalise the relevant trends in  $K$ -value in light of the controlling chemical kinetics, the latter being well understood for idealised reactors [9, 10, 11, 12]. A simple phenomenological engine model which retains the basic physics of SI combustion has been employed to generate representative thermodynamic histories which allow us to explore fundamental aspects which underpin observed trends in  $K$ -value.

The slider-crank model [28, 29] has been used to estimate  $V(\theta)$ , the volume of the cylinder as a function of crank angle, for a cylinder with a bore of 72.5 mm, conrod length 300 mm, stroke length of 80.5 mm, with the isentropic compression-expansion equations used to estimate the gas temperature and pressure for a motoring cycle,  $T_m(\theta)$  and  $p_m(\theta)$ . A Wiebe function is then used to model combustion *via* an estimate of the mass fraction of fuel burned at each crank angle step,  $\chi(\theta)$ :

$$\chi(\theta) = 1 - \exp \left\{ -a [(\theta - \theta_0) / \Delta\theta_b]^{m+1} \right\} \quad (2)$$

where  $\theta_0$  is the spark timing,  $\Delta\theta_b$  is the combustion duration, and  $a$  and  $m$  are constants which are typically empirically-fitted to reproduce engine data.

Here we employ estimates of  $a = 5$  and  $m = 2$ , which have previously been shown to reproduce engine data [28, 29, 30]. The derivation of unburnt gas pressure and temperature,  $p_u(\theta)$  and  $T_u(\theta)$ , from  $V(\theta)$ ,  $T_m(\theta)$ ,  $p_m(\theta)$ ,  $\chi(\theta)$  and the polytropic exponent of the unburnt gas,  $\gamma_u$ , is provided in ESI. Whilst  $\gamma_u$  is temperature dependent, as a further simplification to our model we assume a temperature-independent  $\gamma_u$  of 1.28, which is representative of gasoline/air mixtures in the temperature ranges of interest here [28, 29, 30]. What is important to note within our model is that  $p_u(\theta)$  and  $T_u(\theta)$  evolve along an isentrope controlled by  $T_i$ ,  $p_i$ , and  $\gamma_u$ , and the isentrope can be assumed to be weakly dependent on other parameters, such as spark timing, as illustrated in Figures 1–5 of ESI. The effect of engine speed on the onset of knock has been accounted for in the Livengood-Wu [25] integral:

$$\int_{t_i}^{t_f} \frac{1}{\tau(T, p)} dt = 1 \quad (3)$$

where  $\tau(T, p)$  is the ignition delay time computed at a given crank angle step, and  $dt$  is the time step per CAD, and is  $\propto \text{RPM}^{-1}$ .

$\tau(T, p)$  was computed for stoichiometric fuel-air mixtures ( $\phi = 1/\text{air}$ ,  $\text{O}_2:\text{N}_2 = 1:3.76$ ), at every 0.2 CAD from  $\theta_0 \rightarrow \theta_0 + \Delta\theta_b$ . A TRF mixture with known [31] RON/MON/ $S$  values of 87/84/3 and composition 16.7 vol.% toluene/16.7 vol.% *n*-heptane/66.7 vol.% *i*-octane was used as the test fuel.

Calibration curves were constructed for  $\phi = 1$  PRF/air mixtures with ONs in the range 70–100 with ON increments of 2.0 units sufficient to capture the full range of  $K$ -values observed for the test fuel.

All computations of  $\tau(T, p)$  were carried out using the TRF chemical kinetic model of Andrae *et al.* [26].  $\tau(T, p)$  was computed under constant volume conditions using the the homogeneous batch reactor model of the Cantera package [27], with the energy equation turned on, and  $\tau$  defined as the maximum rate of change of pressure during the course of a simulation. For all fuels/conditions studied, the crank angle degree, temperature, and pressure of autoignition are reported in Tables 1 and 2 of ESI, along with the computed OI and  $K$  values for TRF 87/84.

### 3. Results and Discussion

Figure 1 shows the  $K$ -values computed using the described approach. Three trends appear which directly support observed experimental data.  $K$  is shown to increase with increasing intake temperature [7, 13] and with increasing engine speed [5, 7, 13, 19], and decrease with increasing pressure [18, 19, 21].

The complex chemistry which underpins the varying temperature and pressure-dependent ignition behaviour of sensitive and PRF fuels is described elsewhere [9, 10, 11, 12] and will not be re-iterated here. However, Figure 2 synopsis the differences by comparing the fundamental ignition behaviour of three relevant fuels—a 66.7 vol.% toluene/16.7 vol.% *n*-heptane/16.7 vol.% *i*-octane mixture whose RON, MON and  $S$  values of 98, 87, and 11 have been experimentally determined [31], and the PRF fuels which have equivalent

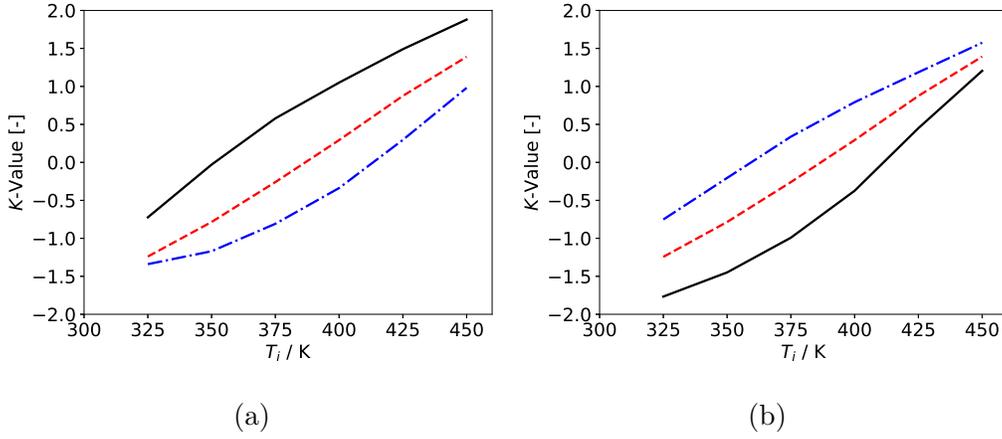


Figure 1:  $K$ -values computed for a RON 87/MON 84 gasoline surrogate as a function of intake temperature ( $T_i$  / K) for (a) intake pressures ( $p_i$ ) of 1.0 (—), 1.5 (---), and 2.0 (— · —) atm at 1000 RPM, and (b) RPM of 500 (—), 1000 (---), and 2000 (— · —) at  $p_i$  of 1.5 atm.

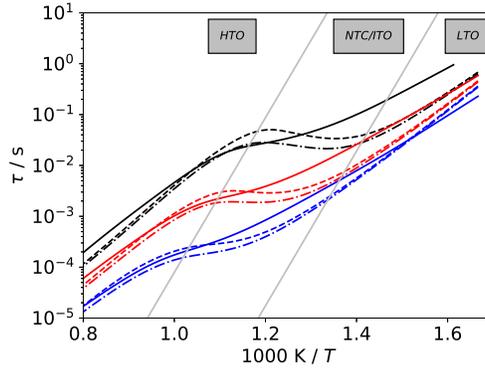


Figure 2: Temperature dependent ignition delay times computed at 10 (—), 40 (---) and 160 (— · —) atm, for a RON 98/MON 87 TRF (—) and its octane-equivalent PRFs; PRF 98 (---) and PRF 87 (— · —). Gray lines demarcate the different ignition chemistry regimes including the low-temperature oxidation (LTO) regime, the intermediate temperature oxidation (ITO)/negative temperature coefficient (NTC) regime, and the high-temperature oxidation (HTO) regime.

RON and MON. This TRF 98/87 mixture was not used in determination of the  $K$ -values as the large vol.% of toluene is unrealistic for a commercial fuel, but its high sensitivity is useful to illustrate and amplify the differences in the ignition behaviour of fuels with sensitivity, and PRFs. In the low-temperature oxidation (LTO) regime, the TRF shows a stronger dependence on pressure than its equivalent RON/MON PRFs, and in the **intermediate** temperature oxidation (ITO)/negative temperature coefficient (NTC) regimes the ignition delay times for the PRFs display little dependence on temperature, in contrast to the TRF.

One of the most interesting and significant features of Figure 2 is that for a given pressure, there is only one temperature condition where the TRF fuel has equivalent ignition delay times to its corresponding RON/MON PRFs. We term these the “RON crossover” and “MON crossover” temperatures, with the temperature of the latter elevated compared to the former. **This trend parallels the elevated intake temperature of the MON test relative to the RON test.** With increasing pressure, the temperature at which the RON and MON crossovers points are observed increases, with the MON crossover point becoming less apparent at very high pressures. The crossover temperatures are significant **as at** temperatures and pressures below the RON crossover temperature, one can expect a sensitive fuel to be more knock resistant than its RON equivalent and the  $K$ -value will be negative. At temperatures beyond the RON crossover temperature, the same fuel will be less knock resistant than its RON equivalent and the  $K$ -value will be positive. What is key is that in practical SI engines, as in subsequent simulations, temperature and pressure are dependent variables, both of which evolve along

a compression isentrope dependent on the isentropic exponent, the intake temperature, and the intake pressure.

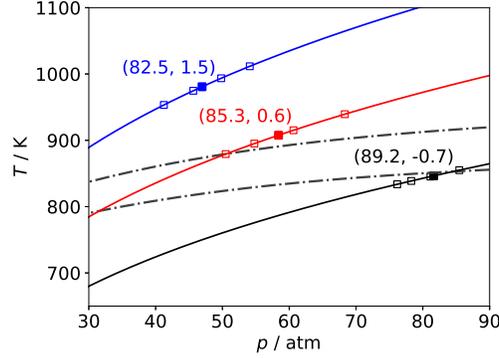


Figure 3: Compression isentropes (solid lines) for simulations with  $p_i = 1$  atm and RPM = 1000 and  $T_i$  of 325 K (—), 375 K (—) and 425 K (—). The temperature ( $T_{auto}$ ) and pressure ( $p_{auto}$ ) at which the Livengood-Wu integral reaches unity are denoted as symbols for a given isentrope. Open symbols correspond to PRFs 72–96 in increments of 8 ON, closed symbols correspond to TRF 87/84. Dashed-dot lines (–·–) indicate the RON and MON crossover temperatures as a function of pressure. Computed octane indices and  $K$ -values are shown in parenthesis.

Figure 3 illustrates the results of engine simulations where  $p_i$  and engine speed are constant at 1 atm and 1000 RPM respectively, but  $T_i$  is varied from 325–425 K. For the  $T_i = 325$  K case, the end-gas experiences a temperature-pressure trajectory which does not transcend the RON crossover temperature before the Livengood-Wu integral reaches unity for TRF 87/84. Under such a trajectory, the ignition delay times of TRF 87/84 which contribute to the Livengood-Wu integral are always greater than its RON-equivalent fuel. The Livengood-Wu integral for TRF 87/84 therefore reaches unity at the same time as a PRF with a RON greater than 87, and the computed  $K$ -value is found to be negative. Increasing the intake temperature to 375 K and 425 K

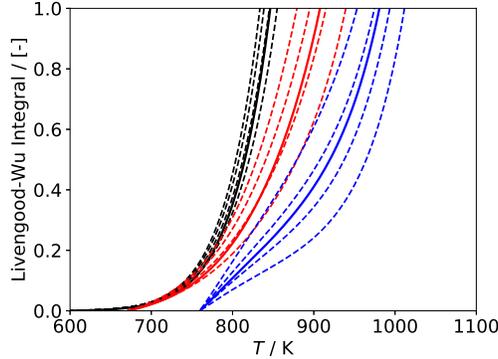


Figure 4: Livengood-Wu integrals as a function of in-cylinder temperature for simulations with  $p_i = 1$  atm and RPM = 1000 and  $T_i$  of 325 K (—), 375 K (—) and 425 K (—). Solid lines correspond to TRF 87/84 with dashed lines corresponding to PRFs 72–96 in increments of 8 ON.

leads to trajectories where the ignition delay times of TRF 87/84 which contribute to the Livengood-Wu integral are at temperatures greater than the RON crossover temperature, Figure 4. The computed  $K$ -values therefore increase as the TRF becomes less knock resistant than its RON-equivalent PRF.

The experimentally observed effects of decreasing  $K$ -value with increasing  $p_i$ , and increasing  $K$ -value with increasing engine speed can be similarly rationalised with an understanding of  $T_{auto}$  and  $p_{auto}$  as shown in Figure 5. Illustrated therein is the dependency of  $T_{auto}$  and  $p_{auto}$  on  $T_i$ ,  $p_i$ , and engine speed for a range of PRFs and TRF 87/84, for four indicative compression isentropes. Also represented are the characteristic RON and MON crossover temperatures for TRF 87/84 as a function of pressure. Those thermodynamic histories which lead to chemical reaction occurring primarily in the low-to-intermediate temperature oxidation regime, where at a given pressure

temperatures are less than the RON crossover temperature, result in negative  $K$ -values for the engine e.g. for  $T_i/\text{K}$  of 350 K and  $p_i$  of 1 atm, and  $T_i/\text{K}$  of 450 K and  $p_i$  of 1 and 2 atm. Similarly, thermodynamic histories where chemical reaction occurs between the RON/MON crossover temperatures will lead to  $K$ -values of 0 to 1, and thermodynamic histories where chemical reaction occurs at temperatures beyond the MON crossover temperature will lead to more positive  $K$ -values. For a given  $T_i$ , an increase in  $p_i$  leads to more negative  $K$ -values as the controlling chemical kinetic behaviour is shifted towards higher pressure and the temperature at which the Livengood-Wu integral reaches unity is decreased. An increase in engine speed will result in increasing  $K$ -values as the temperature at which the Livengood-Wu integral reaches unity is also elevated due to the shorter time interval spent at lower temperatures.

As with many modelling approaches, the current assumptions and results are idealised, but the findings could be of potentially great utility those who desire to correlate the octane requirement of a non-CFR engine with the anti-knock quality of a non-PRF fuel. A much debated presentation [32] at the 36<sup>th</sup> International Symposium on Combustion attempted to define a novel chemical ignition number (CIN) by correlating ignition delay times measured in an RCM, with octane numbers measured in a CFR engine. Whilst this approach is potentially useful, it is clear that any attempt to characterise the ignition quality of a fuel in a modern engine based on ignition delay time measurements in an RCM, shock tube, or similar apparatus, should account for the actual thermodynamic history for the engine condition of interest. Future work should aim to provide experimental verification of

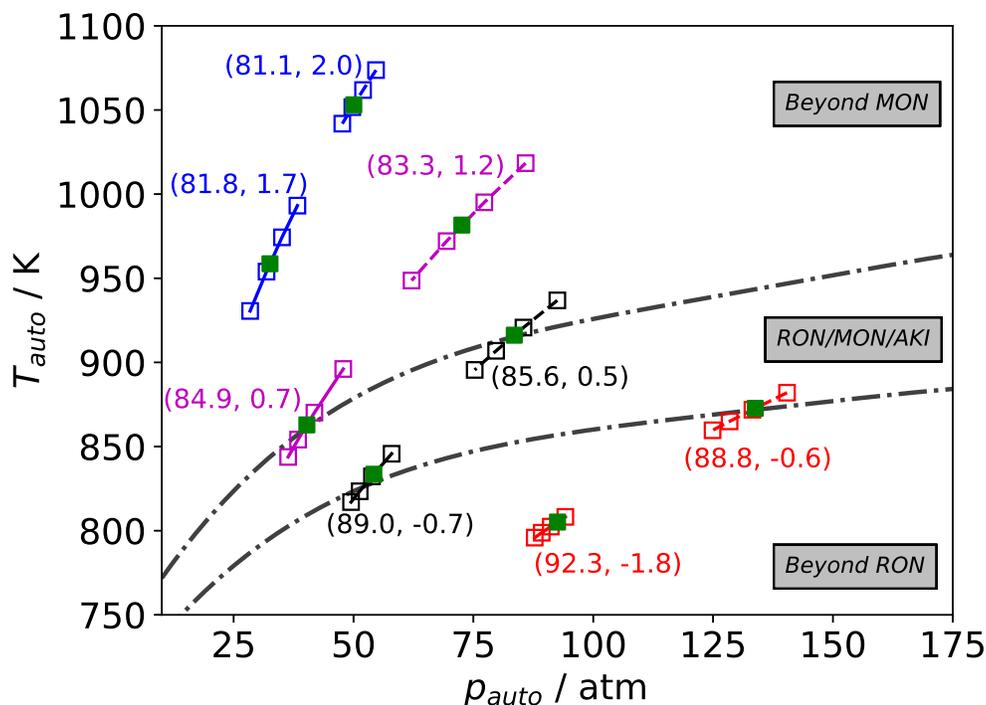


Figure 5: Autoignition temperature ( $T_{auto} / \text{K}$ ) versus autoignition pressure ( $p_{auto} / \text{atm}$ ) for 500 (—) and 2000 RPM (---) cases and four intake conditions:  $T_i = 350 \text{ K}$ ,  $p_i = 1 \text{ atm}$  (—),  $T_i = 350 \text{ K}$ ,  $p_i = 2 \text{ atm}$  (---),  $T_i = 450 \text{ K}$ ,  $p_i = 1 \text{ atm}$  (—),  $T_i = 450 \text{ K}$ ,  $p_i = 2 \text{ atm}$  (---). Open squares ( $\square$ ) correspond to PRFs 72–96 in ON increments of 8 units, with closed symbols ( $\blacksquare$ ) corresponding to TRF 87/84. Dashed-dot lines (---) indicate the RON and MON crossover temperatures as a function of pressure. Computed octane indices and  $K$ -values are shown in parenthesis.

the present interpretation—a series of experiments on well understood test fuels (e.g. PRFs and TRFs) *via* co-ordinated measurements of gas-phase ignition delay times in RCMs and shock tubes, and **efficiency and performance** measurements in CFR and modern engines and vehicles, could allow for improved mapping of octane numbers into chemical kinetic space, and

*vice versa.*

#### 4. Conclusions

Methods which leverage the wealth of scientific knowledge embedded within our present understanding of the RON/MON tests are highly desirable for the design and regulation of next-generation fuels and combustors. The  $K$ -value method of Kalghatgi [5, 6] is one such approach, which allows for the extrapolation and interpolation of measured octane numbers from CFRs to real-world engines. Here, we use a 0-D homogeneous ignition modelling approach to systematically compute and rationalise known trends in  $K$ -value as a function of engine intake temperature, intake pressure, and speed. Computed  $K$ -values are found to reflect experimentally known trends, where  $K$ -values increase with increasing  $T_i$  and engine speed, and decrease with increasing boost pressure. The reported  $K$ -values are interpreted in terms of the underlying fundamental chemical kinetics which occur over the duration of a given thermodynamic cycle, and the computed  $K$ -values are interpreted in terms of ignition chemistry.

Despite the success of the current approach in interpreting known trends in  $K$ -value, there are many other factors which have not been explored in detail in *this work*. It is worth re-iterating that the  $K$ -value modelling approach of Davies *et al.* [14] relies on a measured in-cylinder pressure profile and an estimation of the unburnt gas temperature based on the assumption of an adiabatic-isentropic compression of the end-gas. Figure 7 of ESI illustrates the variations in  $K$ -value due to uncertainties which may arise from the estimation of the unburnt gas temperature, and these are sig-

nificant if temperatures are uncertain by  $\pm 50$  K. Engine and chemical factors which influence the estimation of the unburnt gas temperature such as injection method [21] and charge cooling [33] and exhaust gas re-circulation are worth focusing future experimental and theoretical efforts on. The current approach does not explicitly account for the contributions of flame chemistry and efforts to decouple the contributions of ignition and flame chemistry to knock in engines would allow for a more rigorous understanding of the factors which control RON, MON and  $K$ -value.

## Acknowledgements

Funding from the European Commission Marie Curie Transfer of Knowledge Scheme (FP7) pursuant to Contract PIAP-GA-2013-610897 GENFUEL is greatly acknowledged. KPS would like to thank Dr. Ultan Burke and Mr. Colin Banyon for fruitful discussions on the topic.

## References

- [1] European Commission, Jan. 2013., “Climate Action: Reducing CO<sub>2</sub> Emissions from Passenger Cars”, available at <[http://ec.europa.eu/clima/policies/transport/vehicles/cars/index\\_en.htm](http://ec.europa.eu/clima/policies/transport/vehicles/cars/index_en.htm)>
- [2] W. Zhi, H. Liu, R.D. Reitz, Knocking Combustion in Spark-Ignition Engines. Progress in Energy and Combustion Science 61 (2017) 78–112.
- [3] Standard Test Method For Research Octane Number of Spark-Ignition Engine Fuel. ASTM 2016;D2699-16.

- [4] Standard Test Method For Motor Octane Number of Spark-Ignition Engine Fuel. ASTM 2016:D2700-16a.
- [5] G.T. Kalghatgi, Fuel Anti-Knock Quality - Part I. Engine Studies. SAE Technical Paper 2001-01-3584; 2001.
- [6] G.T. Kalghatgi, Fuel Anti-Knock Quality - Part II. Vehicle Studies - How Relevant is Motor Octane Number (MON) in Modern Engines? SAE Technical Paper 2001-01-3585; 2001.
- [7] V. Mittal, J.B. Heywood, The Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines. SAE Technical Paper 2008-01-2414; 2008.
- [8] V. Mittal, J.B. Heywood, The Shift in Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines Over the Last 70 Years. SAE Int. J. Engines 2 (2) 2010 1–10.
- [9] W. Leppard, The Chemical Origin of Fuel Octane Sensitivity. SAE Technical Paper 902137; 1990.
- [10] C.K. Westbrook, M. Mehl, W.J. Pitz, M. Sjoberg, Chemical Kinetics of Octane Sensitivity in A Spark-Ignition Engine. Combust. Flame 175 (2017) 2–15.
- [11] E. Singh, J. Badra, M. Mehl, S.M. Sarathy, Chemical Kinetic Insights into the Octane Number and Octane Sensitivity of Gasoline Surrogate Mixtures. Energy&Fuels 31 (2017) 1945–1960.
- [12] M.D. Boot, M. Tian, E.J.M. Hensen, S. M. Sarathy, Impact of Fuel Molecular Structure on Auto-Ignition Behavior – Design Rules for Future

High Performance Gasolines, Progress in Energy and Combustion Science 60 (2017) 1–25.

- [13] G.T. Kalghatgi, Auto-Ignition Quality of Practical Fuels and Implications for Fuel Requirements of Future SI and HCCI Engines. SAE Technical Paper 2005-01-0239; 2015.
- [14] T.J Davies, R.F. Cracknell, B. Head, K. Hobbs, T. Riley, A New Method to Simulate the Octane Appetite of any Spark Ignition Engine. SAE Technical Paper 2011-01-1873; 2011.
- [15] T.J Davies, R.F. Cracknell, G. Lovett, L. Cruff, J. Fowler, Fuel Effects in a Boosted DISI Engine. SAE Technical Paper 2011-01-1985; 2011.
- [16] A. Amer, H. Babiker, J. Chang, G. Kalghatgi, P. Adomeit, A. Brassat, M. Gunther, Fuel Effects on Knock in a Highly Boosted Direct Injection Spark Ignition Engine. SAE International Journal of Fuels and Lubricants 5.2012-01-1634 (2012) 1048–1065.
- [17] M. Kassai, T. Shiraishi, A. Teraji, S. Wakefield, T. Goh, D. Doyle, K. Wilbrad, M. Shibuya, The Effect of Fuel Properties on Knocking Performance of Boosted Downsized Engines, Presented at the International Conference “Advanced Fuels for Sustainable Mobility”, 4<sup>th</sup>–5<sup>th</sup> November 2014.
- [18] C.N. Orlebar, A. Joedicke, W. Studzinski, The Effects of Octane, Sensitivity and K on the Performance and Fuel Economy of a Direct Injection Spark Ignition Vehicle. SAE Technical Paper 2014-01-1216; 2014.

- [19] S.M. Remmert, S. Campbell, R.F. Cracknell, A. Schuetze, A. Lewis, K. Giles, S. Akehurst, J. Turner, A. Popplewell, R. Patel, Octane Appetite: The Relevance of a Lower Limit to the MON Specification in a Downsized, Highly Boosted DISI Engine. SAE International Journal of Fuels and Lubricants 7.2014-01-2718 (2014) 743–755.
- [20] A. Prakash, R. Cracknell, V. Natarajan, D. Doyle, A. Jones, Y. Suk Jo, M. Hinojosa, P. Lobato, Understanding the Octane Appetite of Modern Vehicles. SAE International Journal of Fuels and Lubricants 9.2016-01-0834 (2016) 345–357.
- [21] Z. Zhou, Y. Yang, M. Brear, J. Lacey, T.G. Leone, J.E. Anderson, M.H. Shelby, A Comparison of Four Methods for Determining the Octane Index and K on a Modern Engine with Upstream, Port or Direct Injection, SAE Technical Paper, 2017-01-0666 (2017).
- [22] C. Wang, A. Prakash, A. Aradi, R. Cracknell, H. Xu, Significance of RON and MON to a Modern DISI Engine, Fuel 209 (2017) 172–183.
- [23] K.P. Somers, R.F. Cracknell, H.J. Curran, Simulating the Octane Appetite of SI Engines: The Influence of Chemical Mechanisms, Proceedings of the European Combustion Meeting – 2015, Paper P1-68, March 30<sup>th</sup>–April 2<sup>nd</sup>, 2015, Budapest, Hungary, ISBN 978-963-12-1257-0.
- [24] Y. Zhang, K.P. Somers, M. Mehl, W.J. Pitz, R.F. Cracknell, H.J. Curran, Probing the Antagonistic Effect of Toluene as a Component in Surrogate Fuel Models at Low Temperatures and High Pressures. A Case Study

- of Toluene/Dimethyl Ether Mixtures. Proceedings of the Combustion Institute 36 (1) (2017) 413–421.
- [25] J.C. Livengood, P.C. Wu, Correlation of Autoignition Phenomena in Internal Combustion Engines and Rapid Compression Machines, Symposium (International) on Combustion 5 (1955) 347–356.
- [26] J.C.G. Andrae, Comprehensive Chemical Kinetic Modeling of Toluene Reference Fuels Oxidation, Fuel 107 (2013) 740–748.
- [27] D. G. Goodwin, H. K. Moffat, R. L. Speth. Cantera: An Object-Oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes. <http://www.cantera.org>, 2017. Version 2.3.0. doi:10.5281/zenodo.170284
- [28] R. Stone, Introduction to Internal Combustion Engines, 4<sup>th</sup> ed., Palgrave Macmillan, UK, 2012.
- [29] J.B. Heywood, Internal Combustion Engine Fundamentals, McGraw-Hill International Editions, New York, 1988.
- [30] J.B. Heywood, J.M Higgins, P.A. Watts, R.J. Tabaczynski, Development and Use of a Cycle Simulation to Predict SI Engine Efficiency and NO<sub>x</sub> Emissions, SAE Paper 790291 (1979).
- [31] N. Morgan, A. Smallbone, A. Bhave, M. Kraft, R. Cracknell, G. Kalghatgi, Mapping Surrogate Gasoline Compositions into RON/MON Space, Combust. Flame 157 (2010) 1122–1131.

- [32] U. Burke, R.F. Cracknell, M.T. Evans, B. Poulet, S. Gail, I. Kitsopandis, D. Salters, K.A. Heufer, Use of a Rapid Compression Machine to Characterise the Anti-Knock Properties of High-Octane Fuels, Presented at 36<sup>th</sup> International on Symposium, Seoul, South Korea, 2<sup>nd</sup> August, 2016.
- [33] C. Wang, A. Janssen, A. Prakash, R. Cracknell, H. Xu, Splash Blended Ethanol in a Spark Ignition Engine Effect of RON, Octane Sensitivity and Charge Cooling, Fuel 196 (2017) 21–31.