Interpreting Abnormal Combustion Phenomena in Spark Ignition Engines *via* Detailed Chemical Kinetics Modelling

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Un-controlled ignition (knock) has long been recognised as one of the primary-inhibitors in the development of more efficient spark-ignition engines. The anti-knock quality of any petrol fuel is currently defined and regulated based on its associated octane numbers. More specifically, legislation currently specifies allowable limits for research-octane and motor-octane numbers, or RON and MON values, of a given market fuel.

For instance, an "in-spec" EN228 [1] petrol fuel to be sold in the EU must satisfy minimum RON/MON values of 95/85 under directive 98/70/EC, as amended in 2009. Current legislation therefore operates under the general assumption that "the greater the RON and MON of the fuel, the greater the combustion performance", with the latter being defined based on numerous legislated and non-legislated criteria. In truth, there is no single objective criterion for ranking this performance given the complexity of the phenomena which lead to knock.

This in mind, tools *such as* chemical mechanisms (of various complexity) coupled with reactor/engine models (of various dimensionality) can help rationalise the RON and MON values in terms of more fundamental physicochemical properties of the fuel. It is not impossible, that two compositionally different fuel blends with identical RON/MON values might show different responses in terms of *some* performance indicator when used in different vehicles.

Needless to say, the historically-significant (*vide infra*) RON and MON values of a fuel do not encapsulate enough of this underlying complexity to allow one to make a quantitative prediction of how a novel petrol fuel formulation will ultimately perform in real-world engines operating under real-world driving conditions, such as those defined in standard drive-cycles.

The reasons for this are numerous, and can be retrospectively traced to the way in which the RON and MON scales were originally defined. In short, the RON/MON values of market fuels are determined by measuring the crank-angle degree at which the fuel knocks in a co-operative fuels research (CFR) engine which is operating under specified conditions (e.g. speed, load, equivalence ratio, intake air temperature/pressure, etc.). A primary reference fuel (PRF) with a given volume ratio of *i*-octane:*n*-heptane is then blended and tested, until the measured onset of knock is the same as the fuel of interest. By definition, *i*-octane has been assigned *both* RON and MON values of 100 (despite the conditions of the two tests being different), with *n*-heptane assigned values of 0. Hence, the RON/MON values of the real fuel can be derived by knowing the volume ratio of the two components of the PRF blend.

However, there is now sufficient evidence [1–3] to suggest that 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.

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More fundamental approaches to the rational and holistic design of low-carbon fuels for future engines are therefore required, with computational modelling amongst the most promising of these.

From a combustion chemistry perspective, a fossil-derived market fuel could contain hundreds of components, each with their own unique physicochemical properties which contribute to the global combustion properties of the fuel. Thus the historic and continuing need to use simple surrogate formulations based on PRF and toluene reference fuels (TRF), or higher-order blends of *representative components* of the real fuel, to simplify the computational problem.

Indeed, the composition and complexity of the surrogate formulation used to model the real-fuel may vary depending on the property being modelled (distillation curve, ignition delay time, flame speed, [emissions]). The minimum number of components required to accurately model the combustion of petrol fuels is still unclear, but is likely on the order of 5/6/7—a far cry from the binary PRF blends used to determine RON and MON values in the laboratory.

In *this work*, chemical kinetic mechanisms of various complexities (semi-detailed, lumped, reduced) which were designed to replicate the ignition/flame properties of petrol fuels have been used to rationalise the results of experiments gathered in a downsized boosted engine. Simulations using these literature mechanisms dating from 2009–present have been carried out for PRF and TRF blends using a simple 0-D homogeneous reactor model.

The results show that vastly different quantitative and qualitative predictions of knock-onset can arise depending on the mechanism employed. With these results there are obvious implications as to the validity of available mechanisms, where deficiencies in kinetic/thermodynamic input to these models exist, and where experiment and theory can combine to reduce this gap in knowledge. Ultimately the findings contribute to the long-term development of a computational tool which can be applied to the industrial and academic development of Smart Energy Carriers and Technologies.

References

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