

# **Experimental and Chemical Kinetic Modeling Study on the Influence of *n*-butanol blending on the Combustion, Autoignition and Knock Properties of Gasoline and its Surrogate in a Spark Ignition Engine.**

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Engine downsizing, which is aimed at reducing the engine swept volume and consequently fuel consumption without penalising power output, is currently considered as a viable option for achieving a low carbon footprint in the transportation sector. In order for a downsized engine to achieve the same amount of power as the original engine, a boosting system (supercharging) is usually required to increase the density of inlet air. However, supercharging and the use of high compression ratios are currently limited by the phenomena of knock [1]. There is now an increased demand for fuels with high anti-knock qualities as blending agents (octane boosters) [1] and this has also triggered a renewed interest to better understand the autoignition and knock behaviour of new and alternative fuels for the purpose of optimising engine design and control strategies (i.e. ignition timing optimisation). Autoignition and knock in an engine are governed by chemical kinetics and depend on the chemical composition of the fuel and on the evolution of pressure, temperature and equivalence ratio [2]. It would be helpful therefore, to be able to use computer simulations employing chemical kinetic mechanisms of fuels in main engine combustion models to reliably predict and understand autoignition and consequently knock in an engine.

In the past, attempts have been made to predict autoignition using various simple empirical models. Two of such correlations are the popular Douaud and Eyzat (D&E) model [3] derived from the Arrhenius function and the Livengood-Wu integral [4]. In terms of chemical kinetic modelling, the prediction of autoignition in the engine has been limited to the use of very basic global chemical reaction mechanisms developed for a limited number of fuels, e.g. the ‘Shell model’ [5] comprised of 5 species and 8 generalised reactions representing chain/degenerate branching and termination steps, and the skeletal Hu and Keck model [6]. However these global kinetic models, just like the empirical models, have been proven to be grossly inaccurate in terms of agreement with measured data. The various unique features of combustion such as the cool flame and two stage ignition as well as the long ignition delay times exhibited by certain hydrocarbons fuels can only be reasonably explained by the intermediate elementary reactions that make up the detailed reaction mechanism. Therefore the use of detailed or reduced reaction mechanisms that are coupled to main engine combustion models offers a far greater capability to predict autoignition in an engine to a higher level of accuracy and therefore forms the basis for this study. It should be noted that chemical kinetic models are however generally developed and validated within fundamental engine-like setups such as RCM, JSR, shock tubes etc., where the effects of fluid dynamics and turbulence are suppressed [7-9] and where the prevailing *P-T* conditions are much more representative of the *P-T* conditions occurring before autoignition in HCCI and/or controlled autoignition (CAI) engines rather than in SI engines. In

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SI engines, higher  $P$ - $T$  conditions prevail in the end gas due to high compression induced in the end gas by the propagating flame. Therefore it crucial to test the applicability of these models under practical engine conditions in order to establish the impact of the chemistry-flow (fuel-engine) interactions and higher  $P$ - $T$  conditions prevalent in SI engines on the predictability and robustness of these chemical kinetic models. Thus, one of the objectives of this study is to assess the ability of a recently developed reduced TRF/ $n$ -butanol blended mechanism, to accurately predict the autoignition and knock behaviour of gasoline and gasoline/ $n$ -butanol blend under practical SI engine conditions. The detailed model with 1944 species was employed previously in the modeling of the Leeds RCM data [10]. Model reduction was carried out using the method of direct relation graph with expert knowledge, DRG-X [11]. The model was reduced for low temperatures (600-950K), with an error for heat release set at 0.03. Finally, a reduced model with 527 species was generated from the detailed model. A further objective of the study is to link the fundamental understanding developed from the chemical kinetic modelling study within the RCM and presented in a previous paper, with the performance of the TRF/ $n$ -butanol scheme under real engine conditions.

In this work, the impact of  $n$ -butanol blending on the combustion, autoignition and knock properties of gasoline has been investigated under boosted spark ignition engine conditions using both experimental and modelling approaches for stoichiometric fuel/air mixtures at initial temperature and pressure conditions of 320 K and 1.6 bar respectively for a range of spark timings (2 CA- 8 CA bTDC). A formulated toluene reference fuel (TRF) surrogate for gasoline comprising of toluene,  $n$ -heptane and iso-octane has been tested experimentally in the Leeds University Ported Optical Engine (LUPOE) alongside a reference gasoline and their blends (a blend mixture of 20 %  $n$ -butanol and 80 % gasoline/TRF by volume). Although the gasoline/ $n$ -butanol blend displayed the highest burning rate and consequently the highest peak pressures compared to gasoline, TRF and the TRF/ $n$ -butanol blend, it knocked the latest and therefore provides an opportunity for enhancing the knock resistance of gasoline as well as the improvement of the engine efficiency via the use of higher compression ratios. The anti-knock enhancing quality of  $n$ -butanol on gasoline was however observed to disappear at the more advanced spark timing of 8 CA bTDC. While  $n$ -butanol has shown some promise based on the current study, its application as an octane enhancer for gasoline under real engine conditions may be limited. This study would therefore benefit from further experiments and numerical simulations incorporating a wider range of blending ratios. As expected, the TRF fuel showed an earlier knocking boundary of 4 CA bTDC compared to 6 CA bTDC for the rest of the fuels and this was attributed to the absence of an oxygenate (i.e. ethanol or  $n$ -butanol) in the fuel which is present in the rest of the fuels. Knock onset in the end gas computed from the measured cylinder pressure data across the range of knocking spark advance 6 CA - 8 CA bTDC (Figure 1) showed lower knock onsets for TRF compared to gasoline and the blended fuels. Overall, the TRF mixture gave a reasonable representation of the reference gasoline in terms of the produced knock onsets but only at the more advanced spark timing of 8 CA bTDC (Figure 1b) while the TRF/ $n$ -butanol blend gave a fairly poor agreement with the gasoline/ $n$ -butanol blend in contrast to what was observed in the RCM, indicating the need for further studies on the blended fuel.

Similar to the ignition delay time results predicted in the RCM [10], engine simulations of the combustion progress and autoignition tendency of the end gas, performed using the reduced  $n$ -butanol/TRF blended reaction mechanism of Sarathy and the SI model of the LOGEngine code showed that at the lower spark timing of 6 CA bTDC (Figure 2), the predicted autoignition (knock) onsets for TRF and the TRF/ $n$ -butanol blend are higher compared to the measured knock onsets under real engine conditions. The discrepancy between the predicted and measured knock onsets is however quite small at higher  $P$ - $T$  conditions (i.e. spark timing of 8 CA

bTDC). It was also seen in the modelling study that the low-intermediate temperature combustion chemistry within the S.I. engine end gas represented by the presence of a cool flame and NTC phase, plays a very important role in influencing the main or hot autoignition and consequently the overall knock onset due to its sensitisation effect (increasing of temperature and pressure) on the end gas and reduction of the time required for hot ignition to occur. Therefore accurate representation of the low temperature chemistry is crucial for accurate description of the chemical processes and knock occurring within the end gas of an S.I engine. Overall the work provided a link between the ignition delay times predicted in the RCM and the knock onsets predicted within the engine. The work showed that for a mechanism to accurately predict the autoignition characteristics of any fuel under practical engine conditions, it is important that the mechanism accurately reproduces the ignition delay times at the temperature and pressure conditions occurring in the RCM and leading up to the conditions prevalent in the engine.

Keywords: *n*-butanol, autoignition, spark ignition engine, modeling.

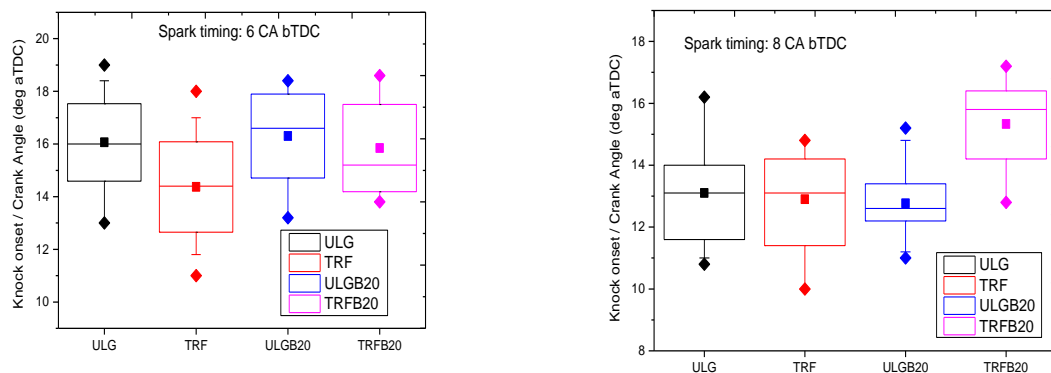


Figure 1: Variation of measured knock onsets across the four fuels tested at (a) 6 CA bTDC (b) 8 CA bTDC. Boxes represent 25<sup>th</sup> and 75<sup>th</sup> percentiles while whiskers represent 5<sup>th</sup> and 95<sup>th</sup> percentiles. The squares and horizontal lines represent the mean and median of the measured distribution.

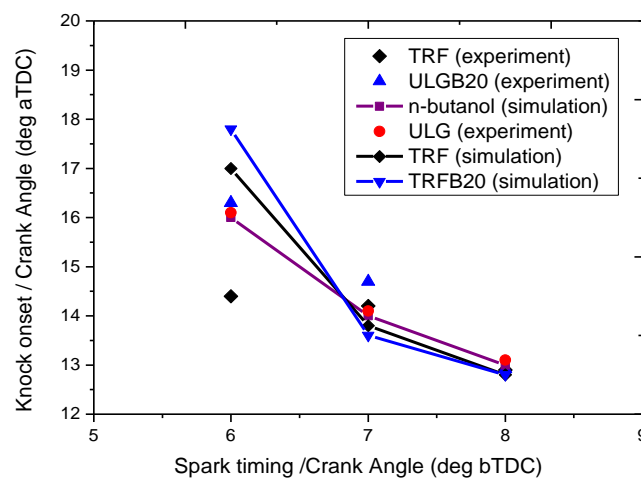


Figure 2: Comparison of predicted and measured knock onsets of TRF blended with 20 % *n*-butanol by volume with those of TRF, gasoline and *n*-butanol.

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