

Investigation of the effects of n-butanol addition to gasoline and its surrogate mixture on the ignition delay times at different blending ratios

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Introduction

Interest in developing alternative clean and sustainable energy has grown substantially over the past decade, driven by the depletion of fossil fuel resources and their environmental costs. Presently, alcohol biofuels, derived from bio-mass and thus being potentially renewable, bio-degradable and oxygenated, are receiving extensive attention from the scientific community. Due to their similar physical and chemical properties to fossil fuels, they are suitable for use as engine fuels or fuel additives in internal combustion engines with little or no modification required, as well as in the current fuelling and distribution infrastructure [1-2]. When added to conventional gasoline, they have the potential of reducing greenhouse gas emissions, as well as offering better knock resistance compared to traditional fossil fuels, thereby improving engine performance.

Ethanol is the most popular choice of liquid biofuel whether used by itself as a neat fuel or blended with gasoline or diesel, attributing more than 90% of the world's total biofuel usage [3]. Butanol is a viable alternative to ethanol and offers several advantages over ethanol, including reduced corrosiveness and high tolerance to water contamination (enabling the use of existing fuel distribution pipelines and longer storage), lower vapour pressure (reducing cavitation, vapour lock problems, evaporative emissions and likelihood of detonation, although making evaporation more difficult), higher energy density (better fuel economy), lower latent heat of vaporisation (decreasing issues with fuel atomisation and combustion during cold start), better miscibility with diesel (higher blending ratios possible), higher cetane number (easier auto-ignition), higher kinematic viscosity (potentially better wear characteristics between moving parts), and a wider range of feedstocks [4-5]. Moreover, its higher heating value combined with the higher stoichiometric air-fuel ratio enables higher blending ratios of butanol in gasoline compared to ethanol without changing regulations with practically no engine modification required, except changes in injection and ignition control strategies [6-7]. On the other hand, the major drawback of bio-butanol is its substantially higher cost of production when compared to bio-ethanol, which is currently preventing it from coming into mainstream use. However, with the development of novel technologies and processes for efficient and economical bio-butanol production, there is a potential for it to cost-effectively compete with bio-ethanol production [8]. Therefore bio-butanol can be expected to become a promising biofuel for spark ignition and compression ignition engines in the future as well as for newer engine designs such as homogeneous charge compression ignition (HCCI).

An important characteristic of any fuel under investigation for blending is its tendency to auto-ignite, which is used in describing the engine startup, emissions, combustion efficiency and knocking. It is therefore paramount to gain a comprehensive understanding of the auto-ignition behaviour of proposed replacement fuels over a variety of operating

conditions. Consequently, the present study investigates the effects of n-butanol addition at different blending ratios to pure gasoline (RON 95 and MON 86.6) and a surrogate gasoline mixture on the auto-ignition behaviour in rapid compression machine (RCM), in particular ignition delay times, through experimental and computational modelling work. Due to gasoline's extremely sophisticated composition of thousands hydrocarbon compounds, it is impractical to develop a detailed kinetic model exactly, therefore a simpler 3-component toluene reference fuel (TRF) surrogate proposed by Agbro et al. [9] has been used in this study for chemical kinetic modelling. The effectiveness of this TRF in representing the ignition delay behaviour of reference gasoline (PR5801 of RON 95 and MON 86.6) when blended with n-butanol at various blending ratios (10%, 40% and 85% by liquid volume) has been examined experimentally to determine its performance in terms of representing gasoline fuel under different blending ratios. Also, to facilitate accurate and efficient predictions of combustion performance, it is important to have a robust chemical kinetic model which can accurately reproduce the desired characteristics of the fuel. Therefore, the robustness in modelling the ignition delay times of the studied n-butanol/TRF blends using a chemical kinetic scheme developed in [9], has been examined here for low the temperature 678-916 K region at a pressure of 2 MPa under stoichiometric conditions. The scheme comprises the LLNL gasoline surrogate mechanism [10] combined with the n-butanol scheme of Sarathy et al. [1] with several updated rate constants as described in [11]. In addition, through the use of local sensitivity analysis, chemical kinetics which governs auto-ignition has been investigated to determine the main reactions which have an effect on the ignition delay times at the end of compression for n-butanol/TRF blends at low temperatures. This would subsequently help to improve the overall understanding of the underlying chemistry involved in n-butanol when blended with gasoline.

Experimental Method

Experiments were performed in the Leeds RCM, which is employed to simulate an ideal single compression stroke of an internal combustion engine and measure the ignition delay times as a function of temperature, pressure and equivalence ratio at constant pressure. It is based on one half of a dual opposed, pneumatically driven and hydraulically damped piston design in which the twin pistons are simultaneously triggered to decrease the compression time and achieve mechanical balance.

Experiments were conducted for 10%, 40% and 85% by liquid volume n-butanol/gasoline blends and n-butanol/TRF blends for temperature range of 678-916 K at 2 MPa pressure under stoichiometric conditions. The mixture composition was determined by measurement of the relative partial pressure and prepared in a separate mixing chamber. Non-reactive runs were also executed for all conditions where the oxygen was replaced by nitrogen, in order to enable variable volume simulations.

Ignition delay time is defined as the time lapse between the end of compression (at TDC) where the piston displacement is zero and the maximum pressure rise rate (dP/dt). Reported ignition delay times are the averages of 4-5 runs made for each test condition with the errors between runs of less than 10% based on one standard deviation.

Computational Modelling

The Cantera software toolkit for a single-zone zero-dimensional engine modelling under Python environment was used to numerically model ignition delay times measured in the RCM by running homogeneous variable volume reactor simulations to precisely mimic the physics of the RCM experiments accounting for the compression phase and heat losses.

The brute force sensitivity analyses were performed at 2 MPa and various temperature conditions using closed homogeneous reactor in Chemkin Pro and constant volume simulations. Temperature sensitivities were first calculated at the time of ignition to identify the most important reactions. The top 30 reactions in terms of normalised sensitivity coefficients were then selected for more detailed analysis. A brute force sensitivity was then conducted for these 30 reactions where the target output was the predicted ignition delay time.

The Influence of n-butanol Blending

Figure 1 shows a comparison between the experimentally determined ignition delay times for the pure fuels (n-butanol, TRF and gasoline) and a blend of both TRF and gasoline with 10% n-butanol by volume. The results show that for the pure fuels, TRF shows similar temperature dependent behaviour to gasoline. However, for the n-butanol/TRF blend ignition delay times lie outside the bounds of unblended fuels in the higher temperature region (765-916 K), when according to a linear blending law they would be expected to lie between the trends of the pure fuels. Only at low temperature conditions (678-702 K) do the two blends illustrate similar behaviour. Therefore, further investigation into the TRF formulation under blending should be carried out. It can be seen that at higher temperatures n-butanol addition to TRF acts as an octane booster giving longer ignition delay times than either of the pure fuels. Interestingly, this behaviour follows only for two temperature conditions of 809 and 782 K for n-butanol/gasoline blend. The negative temperature coefficient (NTC) region is more pronounced for n-butanol/gasoline blend compared to pure gasoline fuel. Again, surprisingly, this NTC region is widened when n-butanol is added to the TRF mixture.

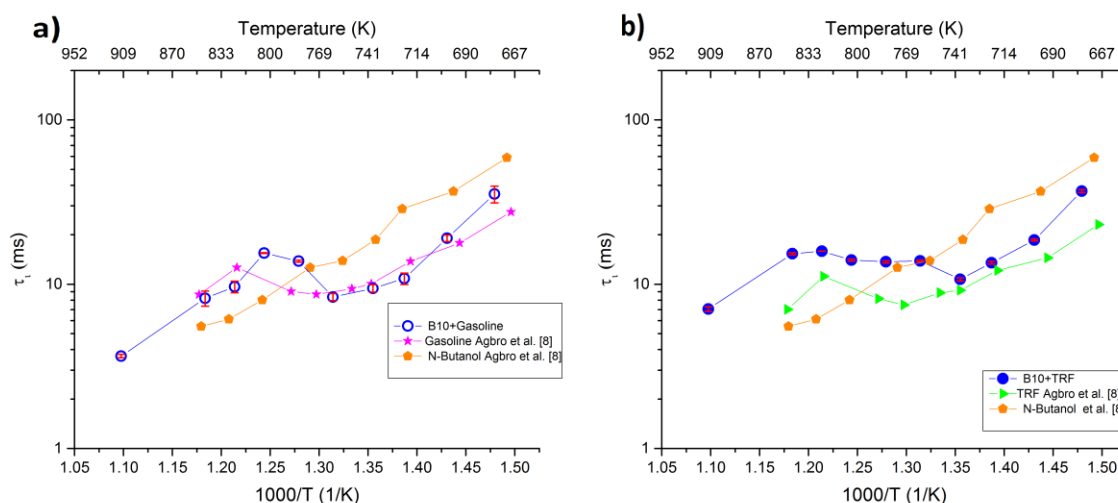


Fig. 1 Experimental ignition delay times for a) gasoline and b) TRF on blending with 10% n-butanol by volume. $P=2$ MPa, $\phi=1$.

The effects of n-butanol addition at different blending ratios to TRF on ignition delay times are shown in Figure 2. It can be seen that at higher temperatures the lowest blend ratio of 10% is acting as more of octane booster compared to any other blend ratios tested in this study. However, within the lower temperature region (678-745 K), an increase in ignition delay times is observed with increasing n-butanol blending ratios showing that n-

butanol acts as an octane enhancer in the low temperature region.

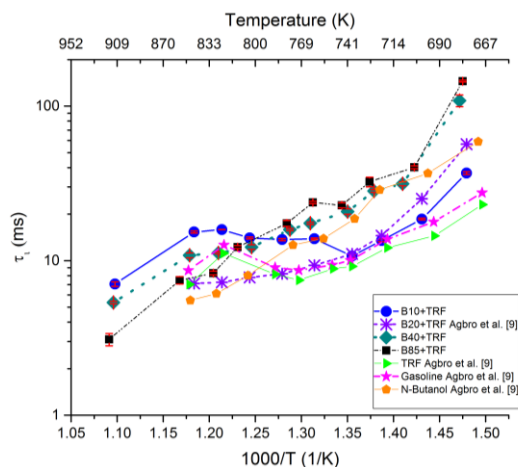


Fig. 2 Experimental ignition delay times for TRF on blending with 10%, 20% (from [9]), 40% and 85% n-butanol by volume in comparison with unblended fuels (TRF, gasoline and n-butanol from [9]). $P=2$ MPa, $\phi=1$.

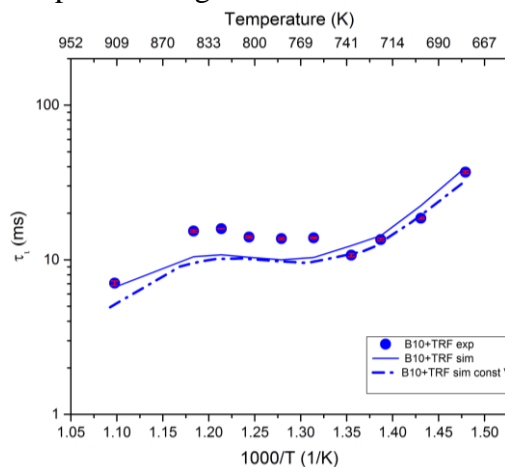


Fig. 3 Comparison of simulated and experimental ignition delay times for TRF on blending with 10% n-butanol by volume. $P=2$ MPa, $\phi=1$.

The ability of the chemical kinetic mechanism to replicate the auto-ignition behaviour for 10% by liquid volume n-butanol blend with TRF is shown in Figure 3. The mechanism captures the general trend of the ignition delay times across the whole temperature range relatively well, only underestimating ignition delay times in the NTC region. However, this could be attributed to experimental errors, as there are many difficulties involved of fulfilling idealised RCM performance and in particular in the definition of NTC region due to non-uniform combustion [12]. Also, constant volume simulations show very close agreement with the variable volume simulations. Therefore, this confirms that constant volume simulation is a viable tool for sensitivity analysis, which would give accurate results with reduced computational cost.

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