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# Influence of Advanced Biofuel Blending with Diesel on the Heat Release, Combustion and Gaseous Emissions Characteristics of a Compression Ignition Engine

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## Abstract

Advanced biofuels are potential low-carbon alternatives to diesel for use in compression ignition (CI) engines. Heat release rates (HRR) and engine emissions may change due to the blending of advanced biofuels. In this study, blends of an alkyl levulinate, a dialkyl ether, and an alcohol were mixed with diesel and tested in a CI engine. Increases in peak HRRs when using the biofuel blends typically correlated with increases in ignition delay times (IDTs). Changes in peak HRR, adiabatic flame temperatures, and charge cooling effects of the biofuel components, influenced nitrogen oxide emissions. Comparisons between gas phase simulations and experimentally observed trends in IDTs highlighted the importance of the physical processes of fuel injection and mixing on IDTs.

## Introduction

Compression ignition (CI) engines are used in the transport, agricultural, and distributed power generation sectors. CI engines are likely to rely on liquid fuels in the near term. To decarbonise these sectors, suitable low-carbon alternatives to petroleum-derived diesel are urgently required. Advanced biofuels are potential low-carbon alternatives and European legislation mandates for an increased use of such fuels [1]. One production process for tailorable advanced biofuel blends from lignocellulosic feedstocks is acid catalysed alcoholysis [2, 3]. The primary alcoholysis products are an alkyl levulinate, a dialkyl ether, and the solvent alcohol [2, 3]. The blends can be tailored to ensure physical property limits in existing fuel standards are met, as well as to maintain or improve engine performance and emissions relative to petroleum-derived diesel.

The addition of advanced biofuel components to diesel results in changes in the combustion behaviour, and as a result the engine performance and emissions [4]. Heat release rates (HRR), in-cylinder pressures, and ignition delay times (IDTs) are combustion properties that typically change upon addition of advanced biofuels [4]. Due to changes in HRRs and IDTs upon biofuel addition, the particulate matter (PM), nitrogen oxide ( $\text{NO}_x = \text{NO} + \text{NO}_2$ ), CO and total hydrocarbon (THC) emissions are likely to change [4].

Frigo et al. [4] showed that with increasing n-butyl levulinate (BL) fractions in blends of diesel, BL, and di-n-butyl ether (DNBE), the suppression of low temperature heat release occurred. This delayed the fuel blends' ignition, along with reducing the peak pressure after ignition, as the ignition occurred further from top dead centre (TDC) [4]. The longer IDTs and delayed heat release from the biofuel blends resulted in increased THC and CO emissions relative to diesel.  $\text{NO}_x$  emissions showed small changes relative to the diesel baseline for most of the blends tested [4]. However, the blend containing 11 vol% BL showed an increase in  $\text{NO}_x$  emissions at all engine speeds and

100% torque compared to diesel, whereas the blends with 7 and 13 vol% BL were more comparable to the diesel baseline [4]. These differences highlight that there is competition between the influences of the different biofuel components. For example, BL has the highest adiabatic flame temperature of the butyl-based blend components (table 1), which could increase thermal  $\text{NO}_x$  production, but requires higher amounts of energy to vaporise due to its high heat capacity and high boiling point [5]. DNBE is known to have a charge cooling effect which can reduce the in-cylinder temperatures and  $\text{NO}_x$  emissions, even with low DNBE fractions [6]. Therefore, the combination of these effects will compete and result in differing effects on  $\text{NO}_x$  emissions for different blend compositions.

Table 1. Combustion relevant physical properties of the fuel components: ultra-low sulphur diesel (ULSD), ethyl levulinate (EL), ethanol (EtOH), n-butanol (BuOH), and diethyl ether (DEE).

Fuel Component	Enthalpy of Vaporisation (kJ/kg) <sup>a</sup>	Heat Capacity (J/kg K) <sup>d</sup>	Adiabatic Flame Temperature (K)
ULSD	250 – 358	-	2200 – 2250
EL	358 <sup>b</sup>	1914 <sup>e</sup>	2875
BL	325 <sup>c</sup>	1962 <sup>e</sup>	2860
EtOH	918	2431	2242
BuOH	702	2401	2450
DEE	366	2361	2300
DNBE	346	2135	2865

<sup>a</sup>from [7-10], <sup>b</sup>at 420 K, <sup>c</sup>at 785 K, <sup>d</sup>from [10], <sup>e</sup>from [11], <sup>f</sup>from [5, 12-14].

Rakopoulos et al. [15] showed that for increasing fractions of DEE, BuOH, and EtOH in diesel,  $\text{NO}_x$  emissions from a single-cylinder CI engine decreased (at indicated mean effective pressures ranging between 1.4 – 5.37 bar). They reported that the addition of 24% DEE to diesel increased the IDTs more than the addition of 24% BuOH, which demonstrates that although DEE has the highest derived cetane number

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(DCN), its volatility can cause issues such as vapour locking preventing fuel delivery to the engine, resulting in longer IDTs [15, 16]. These changes in IDT and emissions may indicate a change in the HRR profile. This dependence of engine-level phenomena on HRR highlights the importance of accurately characterising the influence of biofuel blending on fundamental combustion behaviour.

Simulations provide a useful tool to further the understanding of the influence of changing the blend composition on combustion. Simulations rely on suitable and robust chemical kinetic mechanisms. For new potential advanced biofuel blends with base fuels, such as those used in this work, validated mechanisms are not currently available. However, mechanisms can be produced using automatic generation methods, as discussed by Michelbach and Tomlin [17].

Kim et al. [18] showed through computational fluid dynamic (CFD) simulations of a constant-volume combustion vessel (and subsequent local sensitivity analysis) that changing the heat capacity and density of a fuel had the largest influence on the IDT and HRR. Therefore, with the addition of the biofuel components to diesel, these properties will change and thus influence IDTs and HRRs. This study utilises experimental data and gas phase simulations to investigate the influence of advanced biofuel blending on the combustion, emissions, and heat release characteristics of a CI engine.

#### Methodology

Ethyl-based blends of EL, DEE, and EtOH with ULSD were formulated to achieve stable engine operation and to provide the ability to achieve all five desired engine loads after initial testing found that high fractions of DEE caused unstable operation. Butyl-based blends of BL, DNBE, and BuOH with ULSD were formulated to meet the flash point, kinematic viscosity at 40 °C, and the density at 15 °C limits in the BS 2869 grade II diesel standard [19].

Ethyl and butyl-based blends were tested in a single-cylinder, constant speed, Yanmar L100V engine, with properties detailed in table 2.

Table 2. Yanmar L100V engine specification.

Property	Value
Number of Cylinders	1
Cycle	Four-Stroke
Compression Ratio	21.2
Cooling	Air Cooled
Injection	Direct
Injection Timing (° before TDC)	13.5
Engine Speed (RPM)	3000 ± 100
Maximum Displacement (cm <sup>3</sup> )	435
Engine Power (kW)	0.26 – 5.7

Steady-state engine tests were conducted at five individual loads ranging from 4% to 92%. In-cylinder pressure was measured using an AVL GH14D pressure transducer connected to an AVL FlexIFEM charge amplifier. Pressure-volume and pressure-crank angle

(P-CA) traces were generated using an in-house LabVIEW programme. HRRs were calculated using a modified model based on that of Olanrewaju et al. [20] in order to provide representation of the Yanmar L100V engine. The modifications included the use of a single fuel injection, and the Yanmar engine geometry. The HRR model was derived from the first law of thermodynamics. It assumes the charge is a single zone, zero-dimensional, ideal gas. The model has terms to account for heat losses to the wall, blow-by losses, and evaporative losses. A second order Savitzky-Golay filter was applied with a five point window to reduce the influence of noise in P-CA traces [21]. The effect of the filter on the HRR profile can be seen in figure 1.

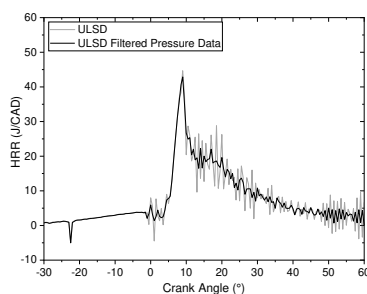


Figure 1. Effects of applying the Savitzky-Golay filter to the pressure data on the HRR curve.

IDTs in the engine were defined as the difference between the start of injection and start of combustion, which is defined as the maximum  $dP/dCA$  after TDC.

Variable volume simulations of ethyl and butyl-based blends were conducted using the closed homogeneous gas phase reactor module in Chemkin 22R1 [22]. Volume profiles from the corresponding 92% load CI engine test were used in the simulations to represent the piston motion of the Yanmar L100V. The simulated IDT was defined as the time taken to reach peak hydroxyl free radical (OH) concentration, which corresponds to the maximum  $dP/dt$ . The simulations enabled the investigation of the extent of the chemical component of the IDT, as only the gas phase combustion was simulated in an adiabatic reactor. The conditions simulated are summarised in table 3.

Table 3. Conditions for the variable volume simulations.

Property	Value
Initial Pressure (bar)	37
Initial Temperature (K)	960 Ethyl-based blends 964 Butyl-based blends
Equivalence Ratio	0.5
Engine Load Represented	92%

The chemical kinetic mechanisms for the ethyl and butyl-based three-component blends were produced in the parallel study of Michelbach and Tomlin [17]. The three-component mechanisms were merged with the two-component diesel surrogate mechanism of Pei et al. [23]. The merged ethyl-based mechanism had 523

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species and 8187 reactions. The merged butyl-based mechanism had 1280 species and 42829 reactions. The diesel surrogate used in this work was composed of 21 vol% m-xylene/79 vol% n-dodecane, as this gave a DCN of 51 when using a linear-by-mole blending law [16]. The ethyl and butyl-based blends tested are summarised in table 4.

Table 4. Fuel blends tested in the engine and simulated. Those highlighted had their HRR analysed.

Blend	Diesel (vol%)	Biofuel (vol%)	Levulinic:Alcohol:Ether (vol%)
Ethyl-1	85	15	75:5:20
Ethyl-2	85	15	95:5:0
Butyl-1	90	10	65:5:30
Butyl-2	90	10	75:5:20
Butyl-3	90	10	85:5:10
Butyl-4	90	10	85:10:5
Butyl-5	90	10	90:5:5
Butyl-6	75	25	85:5:10
Butyl-7	75	25	90:5:5

#### Influence of the Biofuel Blends on the IDTs

IDTs extracted from engine data are influenced by the physical processes of turbulent mixing and fuel vapourisation, as well as the chemical autoignition of the fuel [18]. All of the ethyl and butyl-based blends had longer IDTs than ULSD by up to about 12% depending on the blend composition (figures 2 & 3, respectively).

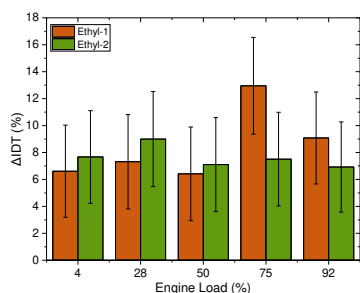


Figure 2. Percentage changes in IDT for ethyl-based blends with respect to the ULSD baseline.

The ethyl-1 (with DEE) had longer IDTs at the higher loads than ethyl-2 (without DEE). This was unexpected, since DEE has the highest DCN of the ethyl-based blends, and thus small volumes of DEE would be expected to act as a DCN enhancer [16]. However, at higher loads, more fuel is injected, hence, the charge cooling effects of DEE are likely to be more potent. For the butyl-based blends at 10 vol% biofuel (butyl 1-5), at the higher loads, there was less of a correlation with the BL fraction in the blend and the increase in the IDT. This could be due to the lower DNBE fraction resulting in less charge cooling, leading to less of an increase in IDT relative to the diesel baseline. The increases in IDT affect both the engine performance and emissions. For example, the longer IDTs could favour a reduction in PM emissions, as

there would be fewer in-cylinder rich zones where PM is typically produced due to there being an increased mixing time [24]. However, there could be an increase in incomplete combustion due to there being less time available for the combustion to occur in the cylinder, which may affect CO and hydrocarbon emissions.

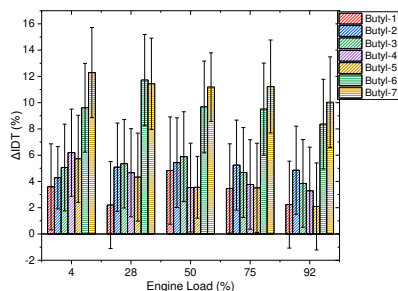


Figure 3. Changes in IDT for butyl-based blends with respect to the ULSD baseline.

#### Simulated IDTs Compared to Experimentally Derived IDTs

Since the chemical kinetic simulations were conducted using a gas phase homogeneous reactor, the simulations could only capture changes due to the chemical properties of the gas phase mixtures. No changes in turbulent mixing could be determined without resorting to costly CFD simulations. Therefore, comparisons between the trends in the simulated changes in IDT with those observed in the engine provide information on the relative importance of the chemical and physical effects of the blend properties. Comparisons were made at 92% load conditions.

Figure 4 shows the differences between simulated and experimental change in IDT relative to diesel ( $\Delta$ IDT) for ethyl-1 and 2. DEE reduced the chemical IDT, as expected since it has the shortest IDTs of the ethyl components [17]. In the engine, there were large positive  $\Delta$ IDTs, which were likely due to increased physical delays [18]. Therefore, the change in chemical IDT was a small portion of the change in total IDT.

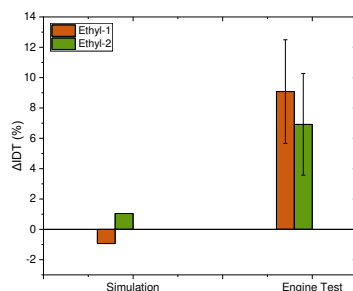


Figure 4. Comparison of the changes in IDT relative to diesel (surrogate for simulations and ULSD for the engine tests) for the ethyl-based blends at 92% load.

The change in simulated IDT of the butyl-based blends, relative to the surrogate diesel, show a strong

correlation to the BL fraction which increases from bButyl-1 up to bButyl-7. This was expected as BL has the longest IDT of the butyl components, as shown Michelbach and Tomlin [17]. In the engine, physical effects also play a role and there is competition between DNBE's high reactivity and its charge cooling effects, and the higher density and heat capacity of BL (table 1). This could explain the drop in  $\Delta$ IDT for the bButyl 2-5 blends as the fraction of DNBE decreases (figure 5). The  $\Delta$ IDT of most blends was greater in the engine than in the simulations. This difference arises because the simulations do not capture changes due to turbulent mixing or injection effects. Simulated  $\Delta$ IDTs show that the increase in chemical IDT could account for around 50% of the increase in total engine IDT. CFD calculations could capture the interaction between chemical processes and physical and mixing effects, but would require heavily reduced chemical mechanisms in order to be tractable.

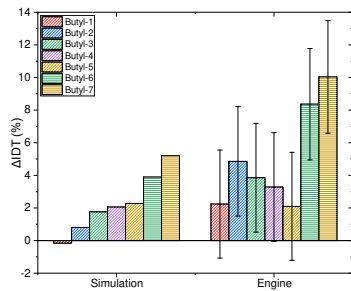


Figure 5. Comparison of the changes in IDT relative to diesel (surrogate for simulations and ULSD) for the engine tests for the butyl-based blends at 92% load.

#### Influence of the Biofuel Blends on HRRs

Analysis of the HRR curves for ethyl and butyl blends (figures 6 & 7, respectively) indicated that the longer IDTs increased the premixed combustion phase, as shown by the larger peak around 10° for most of the biofuel blends tested. The ethyl blend with DEE (ethyl-1) had a lower peak HRR than ULSD and ethyl-2; possibly due to lower in-cylinder pressures resulting from the charge cooling effect of DEE and the reduced injection performance due to vapour locking.

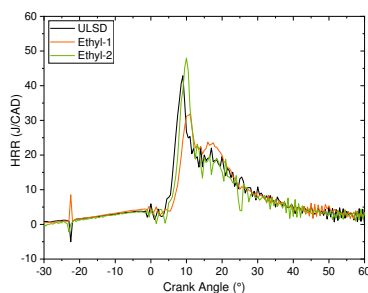


Figure 6. HRRs for the ethyl-based blends and ULSD at 92% load.

The butyl blends had stable operation and their longer IDTs compared to ULSD are evident in the HRR traces (figure 6). Peak HRRs increased relative to ULSD, which correlates to increases in IDTs (figure 3).

There was no evidence of the influence of fuel injection on the HRR at -13.5°. There was also no evidence of vaporisation or charge cooling in the HRR. This is somewhat unexpected, as the addition of the biofuel blend would have changed the enthalpy of vaporisation and heat capacity of the overall blend. However, this lack of an observable change in HRR may have been due to the limited pressure logging resolution of 0.5°.

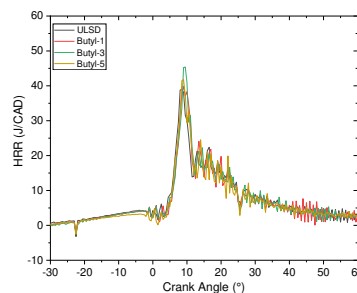


Figure 7. HRR at 92% load for the 10 vol% butyl-based blends and ULSD.

Changes in peak HRRs for the ethyl-based blends can be seen in figure 8. At 50% load, where less fuel is injected, DEE has less of a detrimental effect. There was an increase in peak HRR and this was likely due to increased premixed combustion. However, at 92% load, the blend with DEE had a reduction in peak HRR, which was likely due to instabilities in the engine operation, due to DEE's volatility. This is also evident in figure 4 where the orange curve for ethyl-1 is shifted, as the peak HRR is lower and later in the piston cycle. The lower peak HRR may be beneficial as it would lead to lower in-cylinder temperatures and thus reduce thermal NO<sub>x</sub>. However, the engine may have a reduced thermal and mechanical efficiency as lower pressures and temperatures would be reached during combustion.

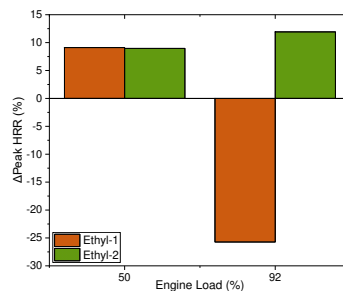


Figure 8. Changes in the peak HRR at 50% and 92% load with the ethyl-based blends relative to the ULSD baseline.

At 50% load, the peak HRR for the butyl-based blends was lower than that of diesel, with the exception

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of the butyl-7 blend, as shown in figure 9. This may have been due to the reduced energy content of the butyl fuel blends. The longer IDT for butyl-7 (figure 3) may have further increased premixed combustion, and thus caused an increase in peak HRR. However, at 92% load the peak HRR increased even with the lower energy content of the blends and the biofuel components (table 1). This increase was likely due to increased premixed combustion because of the longer IDTs (figure 3). The reductions in peak HRR may reduce thermal NO<sub>x</sub> production but may favour incomplete combustion due to lower in-cylinder temperatures and pressures.

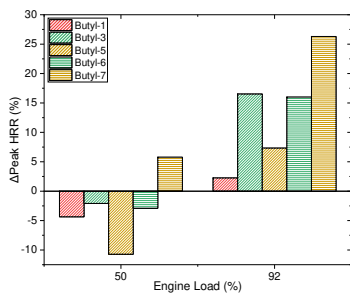


Figure 9. Changes in the peak HRR at 50% and 92% load with the butyl-based blends relative to the ULSD baseline.

#### Influences of HRR on Emissions

Since NO<sub>x</sub> emissions are temperature dependent, the peak HRR and its timing will affect the in-cylinder temperature and thus NO<sub>x</sub> emissions [24]. Increased premixed combustion is also likely to reduce the PM emissions, as discussed by Wiseman et al. [25].

The NO<sub>x</sub> emissions reduced relative to ULSD when using the ethyl-based blends, as shown in figure 10. Although the peak HRR at 92% load with ethyl-2 was greater than with ULSD (figure 8), it was later than the peak HRR for ULSD (figure 6) and further from TDC. Therefore, the in-cylinder temperature was likely to be lower with the ethyl-based blends. Additionally, it is likely that the charge cooling effects of the biofuel components influenced the gas temperature during combustion [18].

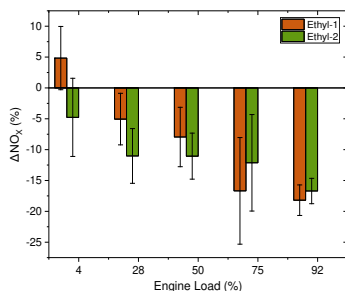


Figure 10. Changes in the NO<sub>x</sub> emissions relative to the diesel baseline for the ethyl-based blends.

For the butyl-based blends the NO<sub>x</sub> emissions are reduced at loads <92% for the blends with high DNBE fractions, as shown in figure 11. At 92% load, butyl-1 produced a reduction in NO<sub>x</sub> emissions, even with a greater peak HRR (figure 9). A possible explanation for this may be that the large DNBE fraction had a greater charge cooling effect due to its high volatility compared to the other butyl-based components (table 1) [18].

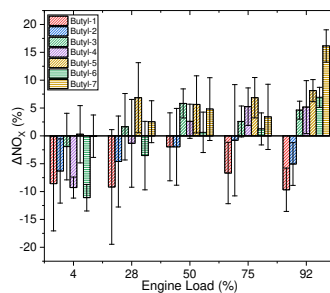


Figure 11. Changes in the NO<sub>x</sub> emissions relative to the diesel baseline for the butyl-based blends.

The increase in NO<sub>x</sub> emissions with butyl-7 may be due to a combination of the greater peak HRR, and BL's high adiabatic flame temperature compared to the other components (table 1), increasing thermal NO<sub>x</sub> relative to ULSD and blends with low BL fractions [24]. Increased engine-out NO<sub>x</sub> emissions could increase the need for exhaust after-treatment systems to control tailpipe NO<sub>x</sub> emissions due to their detrimental impact on local air quality and public health [24] and the need to meet upcoming Euro VII standards.

#### Conclusions

The nature of the HRR profiles of the biofuel blends were not significantly different to those of ULSD. However, the peak HRRs of most fuel blends were seen to influence NO<sub>x</sub> emissions. There may also be some influence from properties such as flame temperatures, which were not measured here. Any optimisation of engine operation to compensate for the longer IDTs would also affect the emissions. The addition of the ethyl and butyl-based blends caused HRRs to change, with higher peak HRRs shown to correlate with longer IDTs. Therefore, the blend composition could be tailored to control the NO<sub>x</sub> emissions whilst maintaining or improving engine performance such as IDTs and HRRs.

Differences between simulated and experimental IDTs show the importance of physical processes such as injection and in-cylinder turbulent mixing. Their contribution to changes in the total IDTs on blending could be as much as 50%. CFD would be needed to capture these effects within simulations, but would require greatly reduced chemical kinetic mechanisms that had been validated over ranges of conditions of relevance to engine operation. Currently, fundamental data suitable for the evaluation of mechanisms for the types of blends studied here is extremely sparse.

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The engine performance and emissions of the butyl-based blends demonstrate that they have the potential to contribute to the RED II target for advanced biofuel use in the transport sector [1]. The blends also show the potential to be low-carbon alternatives to BS 2869 grade II diesel for use in NRMM used in the construction and agricultural sectors [19].

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