**INSIGHTS INTO STOICHIOMETRIC AND LEAN COMBUSTION PHENOMENA
OF GASOLINE–BUTANOL, GASOLINE–ETHANOL, *ISO*-OCTANE–BUTANOL AND
ISO-OCTANE–ETHANOL BLENDS IN AN OPTICAL SI ENGINE**

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ABSTRACT

Introduction of novel fuels such as mixtures of ethanol or butanol with hydrocarbons, requires new fundamental understanding of in-cylinder combustion properties in modern direct-injection spark-ignition engines since those can be quite sensitive to fuel properties. Gasoline and its blends with 25% ethanol and butanol at 25% and 16% per volume (the latter equivalent to 10% ethanol blending ratio in terms of oxygen content) were studied in comparison to gasoline, ethanol and butanol combustion. The same alcohol blending ratios were also employed with *iso*-octane as base component for direct comparison. Testing was performed at 1500 RPM with 0.5 bar intake plenum pressure using 20 °C or 80 °C engine coolant temperature. Thermodynamic parameters were derived using in-cylinder pressure analysis for stoichiometric ($\phi=1.0$) and lean ($\phi=0.83$) fuelling over a range of spark advances. Additionally, high speed colour and greyscale chemiluminescence imaging was conducted at gasoline's maximum break torque spark timing, calculating flame growth speeds, flame roundness and centroid motion. Laminar burning velocity data from the literature and in-cylinder flow measurements from the same engine were used for interpretation. Overall, the analysis showed small differences between gasoline and the blends in general, but showed changes for the pure alcohols with typically much faster flame progression for ethanol and issues with the combustion stability of butanol at low engine temperatures. Alcohol blending, particularly with *iso*-octane, showed some benefits at lean conditions.

INTRODUCTION

BACKGROUND

Combustion of Alcohol Fuel Blends in Engines

Fundamental understanding of the effects of alcohol blending with conventional fuels on in-cylinder spark-ignition (SI) engine processes is of critical importance towards adopting sustainable bio-derived fuel stock. Ethanol is still the most preferred renewable blending component for gasoline. Pump-grade gasoline already contains 5–10% ethanol in many European markets and the US (E5, E10). Such blending ratios are quite compatible with existing fuel systems and, currently, E10 is the legal maximum in many countries for use with standard vehicles (legislation is based on oxygen content). Specially engineered ‘fuel-flex’ vehicles are needed for higher ethanol contents. Ethanol-gasoline blends exceeding E10 have been considered problematic because ethanol tends to concentrate in the lower fractions of gasoline and shifts the distillation curve to much higher volatility than gasoline’s at the lower end of temperatures; this is undesirable as volatility is legislation controlled. Nevertheless, some markets are demanding mainstream blending ratios higher than 10% since low blending ratios can only have limited impact on carbon emissions. In terms of engine design, higher blending ratios are desirable because ethanol has a high Research Octane Number (RON) and high latent heat of evaporation that can enable higher compression ratios for higher thermal efficiency and greater charge cooling for higher volumetric efficiency. However, very high blending ratios can cause problems for cold engine starting due to excessive charge cooling and poor evaporation (Kabasin *et al.*, 2009).

Butanol is a new alternative fuel that carries prospects for wide use in the future; its production processes are already established and despite remaining challenges it is expected that butanol can have similar market share to that of ethanol in the future (García *et al.* 2011; Kumar and Gayen, 2011). Butanol is more compatible with common materials and no major modifications are required to standard refuelling infrastructure processes and fuel injection systems for combustion in engines. Butanol is also less hygroscopic than ethanol, it carries a heating value between ethanol’s and gasoline’s and its RON is very similar to gasoline’s (Owen and Coley, 1995; Gupta and Demibras, 2010). Special interest exists for blends of gasoline with 16% butanol (B16). B16 is similar to E10 in terms of oxygen content. Furthermore, low percentages of butanol blending feature distillation curves not too dissimilar from conventional gasoline grades and hence lower Reid Vapour Pressure (RVP) than ethanol’s blends with gasoline (Andersen *et al.*, 2010a,b). E15 legalisation is being discussed worldwide and this could open the door for legalisation of butanol blends up to ~B25 in terms of oxygen content. E25 may also be a long term possibility if research shows viability.

Several studies of ethanol combustion have been carried out in SI engines with main focus on performance and exhaust emission characteristics. However, most of these involved Port Fuel Injection (PFI) systems (Gautam and Martin, 2000; Gautam *et al.*, 2000; Topgül *et al.* 2006; Nakata *et al.*, 2006; Cooney *et al.*, 2009). Butanol itself has been studied in the literature much less than ethanol and mostly in PFI engines as well; some benefits in terms of blending have been reported (*e.g.* better stability) but trends have been sensitive to equivalence ratio, spark timing, engine temperature and valve overlap (Malcolm *et al.*, 2007; Todd *et al.*, 2010; Szwaja and Naber, 2010; Dernotte *et al.*, 2010; Merola *et al.*, 2011, 2012; Tornatore *et al.*, 2013; Cairns *et al.*, 2013; Deng *et al.*, 2013; Brequigny *et al.*, 2013). In contrast, very few alcohol-blended combustion studies have been conducted in latest technology Direct Injection Spark-Ignition (DISI) engines that are more sensitive to fuel properties than PFI engines. Wallner *et al.* (2009) studied the combustion performance of 10% ethanol and 10% butanol addition to gasoline in a 4-

cylinder DISI engine. Data were taken at engine speeds in the range 1000–4000 RPM. Relatively minor differences were found between all three fuels in terms of heat release rate and combustion stability at low and medium engine loads. Despite efforts that have quantified in-cylinder spray formation and flame speeds in DISI engines using pure ethanol and butanol among other fuels (Serras-Pereira *et al.*, 2008, 2013, 2014; Aleiferis *et al.*, 2010, 2013; Aleiferis and Behringer, 2015), very little information exists on intermediate blends (*e.g.* see Merola *et al.*, 2013 and Irimescu *et al.*, 2015 for B40).

Laminar and Turbulent Burning Velocities of Alcohols

A major aspect of understanding combustion of fuels in SI engines is their laminar and turbulent burning velocities in controlled environments and at engine-relevant conditions. Laminar burning velocities have been measured for a range of liquid hydrocarbon and ethanol fuels at various conditions by Gülder (1984a,b), Metghalchi and Keck (1982), Bradley *et al.* (1998), Jerzembeck *et al.* (2009), Al-Shahrany *et al.* (2005), Liao *et al.* (2007), Bradley *et al.* (2009), amongst others. Data for butanol in comparison to other fuels can be found in Beeckmann *et al.* (2009, 2010) and Gu *et al.* (2009). However, there are differences in values reported by different authors, some of which can be attributed to different measurement techniques, *e.g.* thermodynamic (heat release) *vs.* optical (entrainment), presence of flame cellularity effects at high pressure, the specifics of methodologies used to derive unstretched values of burning velocity, *etc.* Furthermore, the effect of burnt residual gas fraction on laminar burning velocity has not been quantified in detail and very few data exist that are directly relevant to realistic in-cylinder conditions. The overall effect of gas residuals on burning velocities has been quantified as much stronger than that of excess air, temperature or pressure. For example, with residual fractions of 0.15–0.2, the laminar burning velocity of *iso*-octane has been found to decrease by 35–45% according to the seminal work of Metghalchi and Keck (1982). More recently, Marshall *et al.* (2011) published laminar burning velocities at engine-like conditions with and without residuals for both *iso*-octane and ethanol. Vancoillie *et al.* (2011) presented a review of laminar burning velocities and new correlations for the operating range of alcohol-fuelled SI engines. The experimental studies of Broustail *et al.* (2011, 2013) on the laminar burning characteristics of *iso*-octane–ethanol and *iso*-octane–butanol blends at engine-relevant conditions are noteworthy and highly relevant to the present work. The effect of dilution on the laminar burning velocities of *iso*-octane–butanol blends has been addressed by the numerical study of Fu *et al.* (2014). Regarding turbulent burning velocities, limited data exist at engine-relevant conditions for most liquid fuels, including methanol and ethanol (Lawes *et al.*, 2005; Bradley *et al.*, 2011a, 2013), but no data sets exist with residual gas dilution or for butanol fuels. It is also noted that deriving turbulent burning velocities involves several challenges as discussed by Bradley *et al.* (2011b).

PRESENT CONTRIBUTION

No major studies have compared in detail the in-cylinder behaviour of ethanol and butanol blends with hydrocarbon fuels in modern DISI engine configurations. The present study aimed at taking this step by heat release analysis and flame chemiluminescence imaging using 16% butanol blending into gasoline (B16, equivalent to the current limit of oxygen-content legislation), as well as 25% butanol and 25% ethanol blends for direct comparison. Gasoline and the pure components ethanol and butanol were also tested. This was done in a single-cylinder research engine under thermal and optical configuration. The thermal configuration allowed mapping of the engine to identify differences in work output over a range of spark timings. The main objective under optical configuration was to quantify flame speeds, their shape distortion and their in-cylinder motion, the latter in consultation with in-cylinder airflow velocity data from the same engine obtained by Laser Doppler Velocimetry

(LDV) and Particle Image Velocimetry (PIV) (Malcolm *et al.*, 2011; Aleiferis *et al.*, 2016). It was also decided to perform the same work with the same blending ratios in *iso*-octane for direct comparison with the respective gasoline–alcohol blends. This decision was also taken because the laminar burning velocities of ethanol and butanol blends with *iso*-octane of Broustail *et al.* (2011, 2013) could be considered in the analysis of the combustion data from the optical engine. In-cylinder flame chemiluminescence imaging was performed at the Minimum spark advance for Best Torque (MBT) of gasoline for all fuels. This was selected to fix nominally the in-cylinder pressure, temperature and flow at the onset of combustion for all fuels. This practice also ensured engine optical data that could be used for direct comparison with constant volume combustion vessel experiments in the literature where similar methods of flame characterisation have been employed for quantifying laminar and turbulent flame speeds of different fuels ignited at same initial ambient thermodynamic and flow conditions.

EXPERIMENTAL APPARATUS AND PROCEDURES

FUELS

Thermophysical Properties

The gasoline base fuel was pump-grade RON95 without oxygenates. The gasoline–alcohol mixtures B16, B25 and E25 were benchmarked against their base components ethanol and *n*-butanol (*i.e.* E100 and B100). The equivalent *iso*-octane–alcohol blends B16I84, B25I75 and E25I75 were also included in the study. All the single components were of chemical grade purity and all mixtures were splash-blended on a volumetric basis. **Tables 1–2** give an overview of the fuels’ thermophysical properties. Those of the single components at 20 °C and 80 °C were obtained from Yaws (2003). If not specified differently, data for gasoline were taken from product data sheets. The densities were measured for all fuels at 20 °C and mass weighting was used for density estimates at 80 °C that could not be established directly due to the onset of bubbling.

Vapour pressures and distillation curves were measured following ISO 17025, with distillation according to ASTM D86 and vapour pressure according to IP394 to obtain Air Saturated Vapour Pressure (ASVP) and Dry Vapour Pressure Equivalent (DVPE), the latter by a statistical correlation to Reid Vapour Pressure (RVP). The most obvious feature of the distillation curves in **Figure 1** is that E25, B16 and B25 all start lower than gasoline’s but, while the butanol mixtures exceed the recovered volume of gasoline at ~105 °C and ~110 °C respectively, the ethanol mixture surpasses gasoline at ~55 °C. The *iso*-octane–ethanol mixture starts to boil distinctly before any of the two base components and shows a distinct step change past 60% recovered volume towards *iso*-octane which follows until 95%; the last 5% fuel of the recovered volume required even higher temperatures. The *iso*-octane–butanol case exhibited similar behaviour but shifted to higher temperatures. It is also clear from the curves of **Figure 1** that E25’s vapour pressure exceeds significantly that of both base fuels as seen in the values of **Tables 1–2**. Butanol did not show this behaviour; the vapour pressures of B16 and B25 were very close to each other and both lay below gasoline’s and above pure butanol’s. In the case of *iso*-octane as base fuel, the resulting vapour pressures for both ethanol and butanol blends were above their base components; nevertheless, E25’s vapour pressure was much higher than B25’s. Pure butanol, as expected, featured distinctly the lowest vapour pressure. Distillation curves of gasoline blends with ethanol or butanol in Andersen *et al.* (2010a) have also illustrated that low percentage mixtures of ethanol increased the RVP above that of the base fuels, whilst butanol addition to gasoline resulted in RVP between gasoline’s and butanol’s. The RVP of the alcohol-gasoline blends of Andersen *et al.* (2010b) were slightly lower than those measured here; differences can be linked to the specifics of the base gasoline fuel. Similar RVP reduction was found in the present work for the *iso*-octane–butanol mixtures. The RVP

of E25I75 showed good agreement with interpolated data using values at 35 °C from Hull *et al.* (2006) and at 60 °C from Ferrando *et al.* (2010).

Measurements of kinematic viscosity were obtained for all fuels using a Brookfield LV DVIII Ultra SC4-18 viscometer. At 80 °C, some the gasoline-based fuels could not be measured due to onset of bubbling and the values shown in **Tables 1–2** have been based on the reduction seen for the respective blends with *iso*-octane as the latter were measured without any issues of bubbling. Mixing butanol with gasoline increased the kinematic viscosity, however, the values were far below pure butanol's. Ethanol's viscosity was also high at cold conditions; mixing it with gasoline or *iso*-octane improved the situation. Typically the blends had a viscosity that was ~40–70% higher than gasoline's. Values of surface tension were measured using a KRÜSS drop shape analysis DSA100 system. The system did not provide an option for measurements at elevated fuel temperatures. The values for ethanol and butanol were higher than gasoline's and much higher than *iso*-octane's. The blends showed values very close to *iso*-octane's, even lower than gasoline's. For the single components, values at 80 °C were acquired from Yaws (2003) and then estimates were obtained for *iso*-octane's blends with the alcohols using percentage weighting.

Chen and Stone (2011) measured the enthalpies of vaporisation of *iso*-octane–ethanol blends as proxy for gasoline–ethanol blends and found a linear relationship with volumetric mixture percentage. No such information could be found in the literature for gasoline–butanol or *iso*-octane–butanol blends and a similar trend as for ethanol's blends was assumed. The values for specific heat and latent heat were linearly interpolated according to percentages of the base components.

Laminar Flame Speeds

Tables 3–4 show values for the base fuel components and their blends obtained by the studies of Gülder (1984), Beekmann *et al.* (2009, 2010) and Broustail *et al.* (2011, 2013). The values have been averaged over a range of temperatures for easier use. All researchers concluded that lower pressures and higher temperatures increased flame speed but it is apparent that the differences in flame speeds at high pressures and lower temperatures are very small, suggesting that the laminar flame speed is not the factor that restricts the use of the investigated fuels and their blends in engines. It is also noted that according to Beeckman *et al.* (2010) addition of 10% ethanol and butanol to gasoline seemed to reduce the laminar burning velocity below that of the base fuels while that of *iso*-octane's blends remained almost unaffected. Addition of higher quantities of ethanol or butanol to *iso*-octane increased the burning velocity (Broustail *et al.*, 2011, 2013).

RESEARCH ENGINE

A single-cylinder optical research engine was used for the present work. This has been designed and built by MAHLE Powertrain UK on the basis of a serial production 4-cylinder 2-litre 16-valve engine. Details about the engine and the test bed arrangement can be found in previous publications, *e.g.* Malcolm *et al.* (2007, 2011), hence only the most relevant features are described in this section. Important engine parameters are summarised in **Table 5** and a picture of the engine is shown in **Figure 2**. A typical Bowditch piston arrangement with a 45° mirror allowed visual access to the combustion chamber. The top of the Bowditch carried a titanium piston crown holding a circular sapphire window. Piston rings made from Torlon were used and operated unlubricated. The crank and cam shafts were equipped with shaft encoders resolving 1800 increments per revolution. An AVL427 engine timing unit was employed for ignition and injection control, as well as for provision of synchronised triggering for image acquisition and in-cylinder pressure recording. The spark was generated by a triple platinum electrode spark plug powered by a coil-on-plug ignition system. All experiments were done at 1500 RPM engine speed and 0.5 bar

load measured in the intake plenum. This condition represents a typical fuel saving operating point during driving. All timings given in ° CA refer to ‘Crank Angle time equivalent’, with one 1° CA corresponding to 0.111 ms at the 1500 RPM speed used throughout this study. A single-hole swirl-type DI injector was mounted on the side of the combustion chamber between the intake valves. The fuel was supplied to the injector by an alcohol-compatible Heypac GX30 pneumatic pump and regulator; the injection pressure was fixed at 80 bar throughout the current study. The start of injection was fixed in the intake stroke at 60° CA ATDC for ‘homogeneous’ mixture preparation. This was based on earlier work that had optimised injection timing to allow maximum time available for evaporation to ignition timing but also minimise piston-crown spray impingement (Aleiferis *et al.*, 2008).

MEASUREMENT TECHNIQUES

Test and Processing Procedures

Acquisition of pressure and temperature data was realised by a 12-bit National Instruments (NI) PCI-6023E DAQ card capable of a sampling rate of 200 kS/s for 16 channels. Pressure sensors with respective amplifiers for in-cylinder pressure, intake plenum pressure, intake runner and exhaust pressure were used, logged and referenced as needed (Kistler 6041A, 4075A10V39, Kistler 4045A2V39, Kistler 7531, respectively). Their digitisation rate corresponded to 0.2° CA at 1500 RPM. The uncertainty in the signals due to electrical interference was a maximum of 0.05% of the full-scale value for the in-cylinder pressure and 1% of the full-scale value for the intake plenum and other pressures, corresponding to a typical uncertainty of ± 5.0 mbar and ± 10 mbar, respectively. Pressure data were post-processed to calculate the Indicated Mean Effective Pressure (IMEP), amplitude and timing of peak in-cylinder pressure, including mean values and Coefficients of Variation (COV=Mean/RMS). Heat release analysis and calculation of Mass Fraction Burned (MFB) was performed using methods based on Stone and Green-Armytage (1987) and Ball *et al.* (1998) and followed practices of earlier work by the current authors for consistency (Aleiferis *et al.*, 2010, 2013; Serras-Pereira *et al.*, 2008, 2013). All uncertainties involved in acquiring and processing in-cylinder pressure data were carefully considered according to Brunt and Emtgæ (1996). The injection duration was adjusted with each fuel for the required Air-to-Fuel Ratio (AFR) conditions according to a wide-range lambda sensor and AFR1200 recorder. In that respect, the injection pulse length for stoichiometric gasoline and *iso*-octane was 1.26 ms, for butanol this was 1.50 ms and for ethanol much longer at 1.85 ms.

Prior to any optical flame work, thermodynamic engine ‘mapping’ analysis was conducted. Main target was to evaluate the required spark timing for highest Indicated Mean Effective Pressure (IMEP) for all fuels (*i.e.* MBT spark advance). For that study, the engine was run in full metal assembly with engine head and liner coolant temperatures set to 80 °C. The spark timing was swept between 46° and 16° CA Before Top Dead Centre (BTDC) and the in-cylinder pressure, plenum, intake runner and exhaust pressures were recorded along with the plenum and exhaust temperatures. Each sweep was executed three times and each spark timing was evaluated for 213 consecutive cycles after an initial warming up phase during which the engine was run and fired for two minutes. Stoichiometric, $\phi=1$ ($\lambda=1$), as well as lean conditions of $\phi=0.83$ ($\lambda=1.2$) were tested.

Flame Chemiluminescence Imaging

Flame images were acquired through the piston’s optical crown window using the engine’s water-cooled metal liner. Stoichiometric as well as lean mixtures were investigated. The ignition timing was fixed at the MBT spark timing of gasoline, 26° CA BTDC for stoichiometric and 36° CA BTDC for lean conditions to enable nominally the same in-cylinder conditions of pressure, temperature and mean in-cylinder flow for all fuels. Two high-speed cameras were employed within the objectives of this paper. Initially, colour flame images with a resolution of

1024×1024 pixels were obtained at a frame rate of 9,000 frames/s, *i.e.* one image per crank angle, using a Photron Fastcam SA-X camera with internal memory of 8 GB and a Sigma lens with 105 mm focal length. The engine temperature was controlled to 80 °C and the study was done for the base fuels, *i.e.* gasoline, *iso*-octane, ethanol and butanol. Then a monochrome Photron APX-RS high-speed camera with a Nikon 60 mm lens was used with f/8 and a shutter speed set to 1/20,000 s; 9000 frames/s were used again and image resolution was 640×480 pixels. 113 cycles with 60 frames per cycle were recorded. The monochrome images were taken for both hot (80 °C) and cold (20 °C) engine conditions at gasoline's MBT spark timing for all base fuels and their blends, *i.e.* gasoline, *iso*-octane, ethanol, butanol, B16, B16I84, B25, B25I75, E25, E25I750. However, it is noted that the flame images of pure butanol at 'cold' conditions had to be acquired at elevated engine temperatures of 35 °C at stoichiometric conditions and at 45 °C at lean conditions, due to unstable combustion at 20 °C. The higher temperature requirement is believed to be strongly influenced by the poorer atomisation of pure butanol at 20 °C due to its higher viscosity and surface tension (Behringer, 2014).

The fast shutter speed reduced background noise but also led to low combustion luminosity levels requiring small thresholding values for processing. A circular mask with a diameter slightly smaller than the piston window was laid over the original image to remove reflections from the metal housing of the optical crown. Then the image was binarised by thresholding and the flame outlining was obtained. **Figure 3** shows a typical flame chemiluminescence image with a superimposed flame outline as automatically identified. In this image, the intake valves are located at the top, the exhaust valves at the bottom, with the spark plug distinctly visible near the image centre. The flame size was measured and the equivalent flame radius, representing the radius of a circle with an area identical to that of the measured flame area A , was calculated as $r = (A/\pi)^{1/2}$. This practice provided data that could also be used for direct comparison with combustion vessel experiments where similar methods of flame radius growth quantification have been employed for laminar and turbulent flame speed characterisations, *e.g.* Lawes *et al.* (2005). Even though simple, this method is believed to return very similar results to more complex elliptical fittings (Ihracska *et al.*, 2013). The flame's centre-point trajectory was traced in an attempt to link the flame progress with in-cylinder flow. To quantify the flame's general shape distortion, a measure of flame roundness was also calculated. This was based on the degree by which the ratio of area to perimeter converged towards the circular shape, following the relation $4\pi A/P^2$, where A the area and P the perimeter of the flame. A perfectly circular flame returns obviously a roundness of 100%, a square shape 79% and an equilateral triangle 60%. A 'jittery' outlining (if small compared to the flame area) can have little effect on the total area but strong influence on the perimeter and, as such, reduce the roundness factor significantly.

Uncertainties in the image processing methodology were estimated by considering binarised flames. Specifically, the area calculated for a flame was compared to the measured area of the same flame but with an extra pixel added to the equivalent flame radius. This was considered to represent an uncertainty linked to the spatial resolution of the imaging arrangement. The change in the binarised area of a flame due to changes in the threshold was also computed; for small flames about 1–2 mm in radius these uncertainties were found to be about 0.2–0.5% and 8–10% per threshold unit of the nominal equivalent flame radius, respectively. For larger flames at ~30° CA After Ignition Timing (AIT) (corresponding typically to ~5–10% MFB depending on fuel), when considering a wider window of uncertainty of 10 pixels, the uncertainties were about 0.5–2% and 1–2% of the equivalent flame radius. Statistical uncertainties in the typical form of standard deviation of a sample set are dominated in engine datasets

by the degree of cycle-to-cycle variations. This metric was calculated for our in-cylinder flame areas and will be presented in the results section. It is also noted for completeness that, despite known limitations of chemiluminescence imaging techniques (typically associated with line-of-sight integration that masks local flame front structure), comparison of results obtained by flame chemiluminescence and Laser-based planar flame imaging has shown consistent trends between the two techniques when it comes to comparing fuel effects (Aleiferis and Behringer, 2015). This provided further confidence in the validity of the results presented in the current paper by flame chemiluminescence imaging techniques only.

RESULTS AND DISCUSSION

ENGINE THERMODYNAMICS

Table 6 summarises the MBT spark timings of all fuels at $\phi=1.0$ and $\phi=0.83$. Discussion is provided in the following sub-sections.

Base Fuels

Figure 4 shows engine mapping results for the base fuels gasoline, *iso*-octane, ethanol and butanol for $\phi=1.0$ and $\phi=0.83$ at 80 °C engine coolant temperature. Lean results are shown as circles and stoichiometric tests as crosses in the charts. Trend lines have also been included in the graphs to aid interpretation. The behaviour of IMEP was quite flat around its peak location for most cases, indicating its relative insensitivity on spark timing within $\pm 3^\circ$ CA of MBT (IMEP values in **Figure 4** are ‘gross’ but the behaviour of ‘net’ IMEP was the same in terms of trends). Ethanol showed the highest IMEP followed by gasoline, *iso*-octane and, lastly, butanol. The coefficient of variation of IMEP (COV_{IMEP}) was below a typical stability limit of 5% for all base fuels at $\phi=1.0$. The values increased strongly for reduced spark advance. This was more prominent at $\phi=0.83$ for gasoline and even more so for *iso*-octane for which misfiring became clearly audible when ignition timing was retarded beyond 30° CA BTDC. Slightly enriching *iso*-octane to $\phi=0.87$ led to recovery and heat release traces that were similar to those of the other fuels at $\phi=0.83$.

The far right chart in **Figure 4** shows the timing of 50% MFB. This could be used to approximate the fuel’s MBT based on the general rule that optimum spark timing has been achieved when the timing of 50% MFB occurs at about 10° CA ATDC. The graph to the left shows the timing of maximum in-cylinder pressure, a_{pmax} , which can also be used to select MBT based on the general rule that optimum spark timing should return an a_{pmax} at about 15° CA ATDC (Heywood, 1988). MBT was taken as the average of both methods for each fuel and this was also found to rest in the peak region of the respective IMEP charts. It is clear that *iso*-octane required distinctly the largest spark advance of 29° CA, ethanol and butanol the smallest at 25° CA, while gasoline’s MBT was quite close to the latter at $\sim 26^\circ$ CA. This behaviour already indicated a clearly slower combustion with *iso*-octane fuelling. Lean mixtures needed longer spark advance and the spread between fuels increased with *iso*-octane’s MBT at 45° CA, gasoline’s at 36° CA, butanol’s at 34° CA and ethanol’s at 32° CA ATDC.

The specific heat energy supplied, based on identical air mass in the cylinder for all fuels (*i.e.* not accounting for any volumetric efficiency differences that may have occurred from differences in charge cooling effects, *etc.*) was calculated to be 3.01 kJ for butanol, 2.99 kJ for ethanol, 2.92 kJ for gasoline and 2.94 kJ for *iso*-octane per kg air at $\phi=1.0$. Ethanol required similar or slightly later spark timing and featured clearly higher IMEP than butanol and gasoline when compared at fuel-specific MBT spark advances ($\sim 3\%$ and 7% higher, respectively). At $\phi=0.83$ ethanol showed the same IMEP to that of gasoline at fuel-specific spark advances, but had still clearly higher IMEP

than butanol (~5%). The higher specific energy content of the injected fuel per kg air led to the expectation that butanol should perform similarly or better than ethanol. However, it seems that the higher laminar burning velocity of ethanol dominated the in-cylinder processes and the influence of charge cooling may have also played a part (e.g. in terms of volumetric efficiency). Butanol's poorer atomisation can also be associated with some of these effects (Behringer, 2014, Behringer *et al.*, 2014, Aleiferis *et al.*, 2015).

Ethanol–Gasoline Mixture

The addition of 25% ethanol to gasoline resulted in a reduction of IMEP below the values of the individual fuels, as shown in **Figure 5**. The MBT spark timing of E25 was close to that of the constituents with 25° CA for stoichiometric and 35° CA ATDC for lean conditions, respectively. The respective IMEP of E25 at $\phi=1.0$ was ~7% lower than pure ethanol and ~4% lower than gasoline. IMEP differences were lower at $\phi=0.83$ with a change of ~3% compared to its two base fuel components. The COV_{IMEP} of E25 was similar to gasoline's at $\phi=0.83$, showing greater susceptibility than pure ethanol to delayed spark timing. It was, however, less sensitive for $\phi=1.0$ where all fuels had low COV_{IMEP} and a wider range of stable spark timings. The specific energy supplied per unit mass of air was similar for E25 and the base fuels. The air fuel mixing of E25 and gasoline from fuel injection effects should have also been similar on the basis of droplet sizing results (Behringer, 2014; Behringer *et al.*, 2014; Aleiferis *et al.*, 2015). The work output was therefore negatively affected for E25 by other in-cylinder factors.

Iso-Octane–Ethanol Mixture

E25I75 featured an IMEP decrease compared to its constituents in **Figure 6**, yet slightly less than for E25 and its maximum IMEP matched that of *iso*-octane for both equivalence ratios. E25I75 required a slightly delayed spark timing of 28° CA and 41° CA BTDC compared to *iso*-octane's 29° CA and 45° CA BTDC at $\phi=0.1$ and 0.83, respectively. The high COV_{IMEP} for *iso*-octane at lean conditions was reduced by the addition of ethanol to values close to those of the other fuels. The high COV_{IMEP} of *iso*-octane was only slightly improved by the addition of ethanol and the engine was operating close to a typical 5% limit at lean conditions.

Gasoline–Butanol Mixtures

Spark timings for fuel specific MBT were identical for the gasoline-butanol blends and close to gasoline's at 25° CA and 35° CA BTDC for $\phi=1.0$ and $\phi=0.83$, respectively. IMEP values of B16 and B25 were not dissimilar to gasoline's at fuel-specific MBT spark timings (~1% difference at $\phi=1.0$ and ~1.5% at $\phi=0.83$), as shown in **Figure 7**. As mentioned earlier, pure butanol exhibited the lowest IMEP.

Iso-Octane–Butanol Mixtures

Iso-octane–butanol mixtures at stoichiometric conditions showed similar behaviour to the respective mixtures of butanol with gasoline. The mixtures' IMEP values in **Figure 8** were in-between the two base fuels. Adding butanol to *iso*-octane at lean conditions seemed to have a larger impact on IMEP compared to adding ethanol. The high COV_{IMEP} of *iso*-octane was significantly reduced by butanol's addition at $\phi=0.83$ and late spark timing (as opposed to ethanol's addition). The engine ran audibly more stable and misfiring was no longer the issue observed for pure *iso*-octane. The MBT spark timing for B16I84 was identified at 29° CA BTDC for $\phi=1.0$ and at 40° CA BTDC for $\phi=0.82$, while for B25I75 it had to be slightly retarded by 2° CA for both equivalence ratios.

Colour Imaging

High speed colour images of typical cycles of the baseline fuels *iso*-octane, gasoline, ethanol and butanol at lean and stoichiometric conditions are shown in **Figures 9–10** (exhaust valves at the bottom, intake at the top). Certain differences are apparent. For all fuels, the spark was still visible at 5° CA AIT, whilst a distinct flame kernel had developed by 10° CA AIT. The least distinct kernel was that of *iso*-octane, indicating longest initial ‘combustion delay’. From here on, *iso*-octane’s flame was developing visibly slower than gasoline, in clear agreement with the engine mapping results. It featured a less bright flame in predominantly blue-violet colour with fewer yellow bright spots than gasoline.

In comparison to gasoline, ethanol showed a faster flame with a bright yellow flame centre and a thin blue flame border. An orange-yellow flame is typically associated with rich fuel regions and/or droplet diffusion burning during combustion. A greenish coloured flame core with blue flame tip instead of the yellow centre shown here was seen by Catapano *et al.* (2013), who investigated bio-ethanol combustion in a scooter’s engine geometry. The green colour was assumed to be due to copper contained in the grape pomace used for ethanol production. The yellow flame core shown here could be due to poorer atomization and evaporation. Analysis of the combustion using spectroscopy and exhaust emissions regarding particulate matter would give further insights. The yellow colouring, however, appears to go in line with the results of Chen *et al.* (2012), who found highly increasing particulate numbers and mass for increasing ethanol content in gasoline and related that to increased mixture inhomogeneities. Specifically, in contrast to the blue flame of gasoline recorded by Chen *et al.* (2012), a distinct reddish flame core was found for their E85 flames and this was associated with soot formation. This is a clearly different trend to the reduction of particulates seen by Catapano *et al.* (2013) for ethanol in comparison to gasoline. This observation may be due to the higher engine load and higher engine speeds of Catapano *et al.* (2013) (2000 or 4000 RPM) than those of Chen *et al.* (2012) who corresponded to low load operation similar to that of the current work. Such differences in the literature highlight the need for more engine and setup specific investigations before general conclusions can be made from the limited amount of published research and from various engine combustion systems.

Similar flame colouring was seen for butanol but at reduced brightness. If the yellow colour of ethanol was only based on diffusion burning due to poor atomisation, butanol was expected to show this even more. Specifically, the Sauter Mean Diameter (SMD) was up to 50% higher than gasoline’s with the current injector, whilst ethanol’s SMD has been measured in-between gasoline’s and butanol’s (Behringer, 2014). This behaviour appears like a general trend when comparing alcohols and gasoline or *iso*-octane with other injector types as well (Behringer *et al.* 2014, Aleiferis *et al.*, 2015). Therefore, yellow colouring could not only be related to droplet sizes during injection. It may be that ethanol’s excessive cooling inhibited droplet evaporation after the end of injection. It may also be that any remaining of butanol’s larger droplets at ignition timing were more dispersed and lower in number compared to ethanol. The effects may have also been fortified by the larger fuel mass injected for ethanol and butanol to achieve the required stoichiometry. Butanol burned slower than gasoline and ethanol but faster than *iso*-octane. At $\phi=0.83$ all flames in **Figure 10** maintained the pre-described colouring, albeit at lower intensities, and the initial combustion delay increased (least for ethanol), with subsequent combustion slower for all fuels (as discussed in the thermodynamic analysis).

There is scarce information in the literature on the colouring and spectroscopy of ethanol and butanol flames. The studies of Merola and co-workers with butanol-gasoline blends in PFI and DISI engines by flame spectroscopy (Merola *et al.*, 2012, 2013; Tornatore *et al.*, 2013) have revealed that, although addition of 40% butanol to gasoline led to decreased emission intensity in comparison to gasoline after TDC, during the early phases of flame development in a DISI engine the B40 blend exhibited higher intensity at the bands of OH and CH excited radicals (308 and 430 nm), as well as stronger broadband background emission from 350–500 nm.

All fuels, including the mixtures, exhibited ‘clipping’ by the boundary of the optical piston crown window around 20° CA AIT at stoichiometric and between 25–30° CA AIT at lean conditions. The vast majority of the flames were progressing in the direction of the exhaust valves first and featured an elongated shape along the pent-roof. The in-cylinder charge flow motion, forward tumble of 5–7 m/s from intake to exhaust, and the two counter rotating swirl vortices under the intake valves (Aleiferis and Behringer, 2015) would have contributed to this behaviour; this is discussed quantitatively in more detail later.

Enflamed Area Growth

The graphs in **Figures 11–12** show the percentage of the piston crown’s window area occupied by the averaged enflamed area against° CA AIT for gasoline and *iso*-octane alcohol blends, respectively. Lean conditions are given in the left graphs and stoichiometric conditions in the right graphs with cold engine conditions (20 °C) at the top and hot engine results (80 °C) in the bottom graphs. The pressure traces that were recorded at spark conditions equivalent to those used for flame chemiluminescence imaging have been included along with their respective MFB curves in the **Appendix** for completeness and for the aid of modellers. A value of 100% in **Figures 11–12** signifies that the flame has covered the whole piston window area. It is noted that the flame area shown in those graphs needs to be studied primarily over the time that the flame remained totally within the optical piston window area. Typically, window clipping started at roughly 30% window area (equivalent flame radius of ~14 mm), between ~20–25° CA AIT for stoichiometric and ~25–30° CA AIT for lean conditions, as indicated by the dashed red line in the graphs. The respective MFB at the clipping point was below 5%. For any flame area comparisons after the timing of initial window clipping, it has to be considered that some flames (especially those of ethanol) showed a more centralised flame kernel and rounder shape so that the occupied optical piston crown area would increase more than that of a gasoline flame that had a higher percentage of flame beyond the boundaries of the optical piston crown. The values of respective standard deviation have been plotted independently in **Figures 13–14**. It is reminded that pure butanol did not fire at 20 °C engine coolant temperature but at 35 °C for $\phi=1.0$ and at 45 °C for $\phi=0.83$, which means that direct comparison at ‘cold’ engine conditions needs to be applied with caution for this fuel. Mixtures containing 16% or 25% butanol exhibited no such limitations.

Pure ethanol showed the fastest flame area growth at all conditions. At hot stoichiometric conditions, ethanol reached the clipping point about 3° CA earlier than gasoline, in relative agreement with the pressure-based heat release analysis behaviour. At hot and cold stoichiometric conditions, gasoline and butanol showed similar flame growth. However, at hot lean conditions, butanol burned faster than gasoline; this is consistent with the MFB analysis discussed earlier. At cold lean conditions, butanol was slower than gasoline.

E25’s performance was between the constituents, with the exception of the hot stoichiometric case, where it was closely mirroring gasoline. The gasoline–butanol mixtures showed similar behaviour and were for hot lean conditions slightly closer to gasoline whilst they followed very similar trends to those of the traces of gasoline and

butanol at hot stoichiometric conditions, 80 °C (similar to the MFB trends). E25 was burning faster than B16 and B25 only at the $\phi=0.83$, 80 °C settings, while little difference was visible at the other conditions.

Out of all fuels, *iso*-octane was the slowest at $\phi=1.0$, 80 °C (as for the MFB trends), but faster than gasoline at $\phi=0.83$, 80 °C. The latter was not in accordance with the thermodynamic analysis but it was a consistent trend and issues of heat losses from the optical configuration of the engine may have been accountable for; this and is clearly an area that requires further focused study (see also **Appendix** on thermal vs. optical engine heat release analysis). At cold conditions, gasoline was always faster than *iso*-octane. The mixture of ethanol with *iso*-octane featured flame areas in-between the pure components but distinctly closer to *iso*-octane. The mixtures of *iso*-octane–butanol were typically burning faster than *iso*-octane except at $\phi=0.83$, 20 °C, where B25I75 appeared distinctly delayed compared to B16I84 which was above *iso*-octane at this condition and similar to E25I75 throughout. The standard deviation of the flame area at the timing of initial clipping was typically between 10–18% at $\phi=0.83$ and 6–15% at $\phi=1.0$. Ethanol was clearly associated with the lowest levels of variability at hot conditions, while butanol was typically the most variable, especially at the lean cold engine operating conditions ($\phi=0.83$, 20 °C).

A measure of initial ‘combustion delay’ was quantified for all fuels and conditions by the first significant rise in area growth rate dA/dt . The values obtained were lower than those derived from the early MFB increase, showing the sensitivity advantage of the optical analysis, typically between 5–7° CA for all fuels at $\phi=1.0$ and in the range 10–15° CA at $\phi=0.83$. For comparison, the integral time scale in this engine was measured to be about 13°–18 CA at the timing of spark, 26° CA BTDC (Aleiferis *et al.*, 2016), and may be linked to the observed combustion delays. Ethanol and butanol showed little sensitivity in their early flame area gradient at both 20 °C and 80 °C for $\phi=1.0$ and at 80 °C for $\phi=0.83$. At cold lean conditions though both alcohols featured increased delay. The hydrocarbon fuels and their blends exhibited generally a stronger initial delay at $\phi=0.83$.

Flame Radius Growth Rate

From the flame area, an equivalent flame radius was deduced and then a flame radius growth rate dr/dt was calculated for each crank angle interval for each cycle and then averaged over all cycles. The graphs of this radius growth rate, *i.e.* the flame expansion speed, are shown against crank angle in **Figure 15** for the gasoline–alcohol blends and in **Figure 16** for the *iso*-octane–alcohol blends. These depict an initial speed greater than zero with declining magnitude until stabilisation at the onset of self-sustained combustion. This feature was more distinct at lean conditions and caused by the strong spark illumination during the very early formation of the kernel. The flame growth speeds generally grew approximately linearly during combustion until they reached a peak value when the flame boundaries started to locally exceed the piston crown’s optically accessible area. It is unclear for how long the almost linear velocity increase would have continued before the flame’s extinction onto the liner walls. The successive decline in flame speed velocity past the peak is due to the flame’s area growth outside the piston window and bears limited quantitative significance but it has been retained in these graphs for relative comparisons between fuels.

Ethanol showed the earliest start of combustion for both 20 °C and 80 °C at $\phi=1.0$ and for 80 °C at $\phi=0.83$. At hot stoichiometric conditions, butanol and the gasoline–containing fuels followed shortly afterwards, slightly earlier than the *iso*-octane-based fuels. Hot lean conditions showed a greater spread between fuels in relation to the onset of combustion, with gasoline trailing last. Despite gasoline being the slowest at these conditions, it achieved a similar peak value speed to the other fuels. At lean conditions, flame speeds were about 20–30% lower than for

$\phi=1.0$. Cold conditions showed generally lower spread between the fuels; all fuels were typically within $\sim 2^\circ$ CA. Ethanol was again among the quickest fuels and butanol was distinctly delayed (despite the higher engine temperatures of $35\text{--}45^\circ\text{C}$), especially at lean conditions. The alcohol mixtures performed typically in-between their base constituents. However, at hot stoichiometric conditions all mixtures were very similar to gasoline or *iso*-octane. In this case, the gasoline–alcohol mixtures did not shift significantly towards pure ethanol, unlike when at cold stoichiometric conditions and for both 20°C and 80°C at $\phi=0.83$ where alcohol addition to gasoline increased the speed of combustion. Despite averaging, some oscillations are still visible on the flame speed traces of some fuels at cold engine conditions, highlighting the lower combustion stability, especially for $\phi=0.83$.

When plotting the flame growth rate against flame radius in **Figures 17–18**, the initial combustion delay is being effectively removed and the speeds can now be compared at the same flame size for all the different fuels. This was required as increasing flame radii return higher propagation speeds associated with the increasing amount of turbulence scales interacting with the flame front and the greater turbulence intensity that the flame gradually ‘sees’ (Lawes *et al.*, 2005). The increase in pressure with ongoing compression has a counteracting effect on the flame speed, but the temperature dependency is typically much greater and compensates pressure-related effects (Metghalchi and Keck, 1982; Gu *et al.*, 2009). When plotting the velocity against a common flame radius, the corresponding crank angles were different amongst fuels, typically within 5° CA at $\phi=1.0$ and up to 10° CA at $\phi=0.83$, with the according effect from in-cylinder pressure and temperature still mostly related to motoring compression during early flame kernel growth. The recorded peak values of the flame speeds in **Figures 15–18** have been summarised for all fuels in bar chart form in **Figure 19**. When weighted by the ratio of burned to unburned gas densities, the peak flame burning velocities were about 7–8 times higher than the laminar burning velocities of the fuels.

At $\phi=1.0$, 80°C , a steep speed gradient was prominent for ethanol over a radius change from 1–3 mm. In succession, ethanol’s flame speed was consistently ~ 1.2 m/s above that of the other fuels at the same flame radius, but the flame’s acceleration was similar to the other fuels. The latter would suggest that most of the advantage in flame propagation found for ethanol was based on a very fast very early flame kernel growth for radii up to 2 mm, *i.e.* at flame diameters just about the same size as the measured integral length scale of turbulence in the vicinity of the spark plug in this engine (~ 5 mm, Aleiferis and Behringer, 2015). The higher laminar burning velocity of ethanol is clearly dominant at these early stages of flame development but the very high flame stretch for ethanol at such small flame radii along with its comparably lower Lewis number (detailed later), may well be contributing to the differences observed.

At $\phi=1.0$, 20°C , the spread between fuels was slightly larger, with gasoline and *iso*-octane showing slowest flame speeds at fixed radii. At $\phi=0.83$, 20°C , ethanol was no longer offset from the other fuels. Noteworthy is the effect of 25% ethanol addition to gasoline at $\phi=0.83$, 80°C , which increased the flame growth speed at fixed radius towards the level of pure ethanol. This effect was not visible for E25I75 though.

Direct comparison of the flame speeds in the engine with turbulent burning data in the literature from combustion vessels with controlled levels of turbulence is not always easy due to the dependency of flame speed on the flame radius and turbulence intensity characteristics (u'). Comparison needs to be done at a similar flame diameter to turbulent length scale ratio. In this context, comparison with the *iso*-octane data of Lawes *et al.* (2005) was possible. Specifically, the latter authors presented turbulent flame speeds at 30 mm flame radius for an integral

length-scale of 20 mm and $u'=2$ m/s at initial conditions of 5 bar and 360 K. This was about 140–190 K lower than the temperature at ignition timing of the current experiments (with an additional ~ 40 K per 10° CA AIT due to continuing compression – quantified by the pressure trace and polytropic index). The required flame diameter to integral length scale ratio for comparison was 3 and based on the integral length-scales of 4–7 mm recorded in-cylinder at ignition timing (Aleiferis and Behringer, 2015), this would require a flame radius of ~ 6 mm for the smaller scales. When correcting the flame speed by the density ratio of unburned to burned gases, the turbulent burning velocity for *iso*-octane at 6 mm radius would be 1.8 m/s for $\phi=1.0$ and 1.45 m/s for $\phi=0.83$ (80 °C engine coolant temperature). These values are roughly double those reported by Lawes *et al.* (2005), who found ~ 0.9 m/s at $\phi=1$ or ~ 0.7 m/s at about $\phi=0.83$. The strong influence of initial temperature is believed to be the cause of different values. Metghalchi and Keck (1982) for example showed that the laminar burning velocity of *iso*-octane approximately doubled when the temperature was increased from 360 K to 550 K for lean and stoichiometric mixtures, at pressures between 0.4–2 bar. It is also noted that the residual gas fraction in this engine was estimated at a modest 7%, yet this would still have an effect on the flame speed. Marshall *et al.* (2011) for example showed a reduction in *iso*-octane's laminar burning velocity from 90 cm/s to 60 cm/s when the residual mole fraction was increased from 0% to 10% at 550 K and 10 bar.

Ethanol, butanol, *iso*-octane and their mixtures were investigated by Broustail *et al.* (2011, 2013) with the conclusions that the laminar burning velocities of the *iso*-octane–alcohol blends typically increased with alcohol content. Laminar burning velocities for the single components were given amongst other conditions at 5 bar, 423 K. Stoichiometric *iso*-octane was burning at 0.36 m/s and at 0.29 m/s for $\phi=0.8$, while ethanol and butanol were both $\sim 17\%$ higher at 0.42 m/s for $\phi=1.0$ and at 0.325 m/s for $\phi=0.8$. This correlates well with the relative differences observed in the current investigation, showing 19% higher maximum turbulent flame speeds for ethanol compared to *iso*-octane; butanol was only higher by 7% though and this can be attributed to poor atomisation and mixture preparation effects. The laminar burning velocities for the *iso*-octane–alcohol blends were presented at 423 K but at 1 bar only. The velocity increase was linear for butanol addition at equivalence ratios ϕ between 0.8–1.2, while the effect of ethanol's addition showed a more progressive increase for $\phi=0.9$ –1.3; the obtained data even showed a slight reduction of the burning velocity for mixtures of 25% ethanol, for $\phi=0.8$ and 1.4. The stoichiometric values for ethanol and E25I75 were 0.65 m/s and 0.56 m/s respectively, whilst for $\phi=0.8$ a value of 0.51 m/s was shown for ethanol and 0.43 m/s for E25I75. The respective values for butanol were 0.62 m/s at $\phi=1$ and 0.51 m/s for $\phi=0.8$. B25I75 showed 0.56 m/s at $\phi=1$ and 0.43 m/s at $\phi=0.8$. In turn, *iso*-octane was close to the mixtures with 0.55 m/s at $\phi=1$ and 0.45 m/s for $\phi=0.8$. These trends appear in good agreement with the current results at 80 °C engine coolant temperature, which show that E25I75 was burning slower at $\phi=0.83$ than pure *iso*-octane and the butanol mixtures were close to the hydrocarbon fuels. The stoichiometric mixtures all showed a slight increase in flame growth speed compared to *iso*-octane; pure ethanol was significantly faster. Also, for the maximum recorded value of flame speed in the engine, typically occurring at radii of 11–13 mm, a distinct increase was found by the addition of 16% and 25% butanol to gasoline or *iso*-octane, as shown in the bars of **Figures 19**. The addition of 25% ethanol to either of the hydrocarbon fuels (E25, E25I75) showed no significant change in peak flame speeds, except for gasoline at $\phi=0.83$, 80 °C.

Figures 20–21 give an estimation of the stretch experienced by the flame in the form of $(2/r)(dr/dt)$. Very high initial stretch rates, typically as high as $6\text{--}7\text{ ms}^{-1}$, were recorded for radii smaller than 1 mm. These high stretch

rates require the support of the spark's energy input to avoid extinction. For $\phi=1.0$ the stretch rate reduced almost linearly for flame radii of 2–10 mm from levels of 3–6 ms⁻¹ to about 2 ms⁻¹ and was, therefore, significantly above usual extinction levels found in combustion bomb experiments (e.g. *iso*-octane at stoichiometry of ~0.5 ms⁻¹, Bradley, 2009). The results showed that there were only small differences among fuels, with the exception of ethanol that exhibited generally the highest levels. In contrast, *iso*-octane was mostly associated with the lowest stretch rates and butanol was intermediate. The effect of engine temperature was relatively small in terms of absolute values but the separation between fuels was clearer at 20 °C with differences among them in the range 0.2–0.5 ms⁻¹ and early stretch rates generally higher than at 80 °C; ethanol showed higher initial stretch at 80 °C though. Lean conditions exhibited lower levels of stretch, with initial levels at radii of 2–3 mm typically lower than 3 ms⁻¹. The work of Brequigny *et al.* (2013) has also shown slower flame growth speeds for *iso*-octane than for butanol but small differences between the stretch rates experienced by the two fuels (albeit at slightly different conditions to those of the current study, namely 1400 RPM, 0.7 bar intake pressure).

Flame Roundness

The analysis of the flame's roundness should provide information regarding the general flame shape distortion and wrinkling. The change in flame roundness during the flame's development at hot engine conditions is given against the flame radius in **Figure 22** for the *iso*-octane-based fuel blends. At the early stages of combustion, just after ignition timing, the roundness successively increased until a maximum at a radius of ~1–2 mm where the flame is believed to be least affected on a macroscopic level by the turbulence intensity inside the cylinder. After this phase, the flame is gradually subject to more distortion by the in-cylinder flow structures whilst encompassing different eddy sizes and this leads to decreasing roundness levels beyond radii of 2 mm. As expected, past the onset of flame clipping by the boundaries of the optical crown (~14 mm flame radius), the flame's roundness converged quickly towards 100% due to the circular shape of the piston window. For lean conditions, the roundness remained approximately constant between 4–14 mm. **Figure 23** summarises the flame roundness at a flame radius of 10 mm for all fuel blends. It is clear that stoichiometric conditions always returned higher roundness and that the hot engine was also associated with rounder flames than at cold conditions. All fuels were typically within 5–10% and no distinct difference between the faster progressing fuels could be seen on the scales involved. The graphs also indicate that the addition of butanol and ethanol to gasoline at stoichiometric conditions slightly increased the flame roundness above that of the baseline fuels. The flames of *iso*-octane at cold conditions displayed clearly the smaller roundness. Blending *iso*-octane with ethanol and butanol led to greater flame roundness, especially at cold engine conditions.

Flame Centroid Motion

The position of the flame's centroid can depend on several factors simultaneously present in-cylinder at ignition timing and competing against each other. These include primarily flame 'convection' by flow motion but the level of spatial fuel concentration/homogeneity and associated temperature and residual gas fields also play a role. The flame centroid locations showed strong cyclic variation, as illustrated in **Figure 24** that depicts the centroids for stoichiometric gasoline at 15 °AIT for 113 consecutive cycles. This figure also shows the flow field measured at ignition timing by PIV (Malcolm *et al.*, 2011; Aleiferis *et al.*, 2016).

The average flame centroid path motions are presented in **Figure 25** for gasoline and its alcohol blends and in **Figure 26** for *iso*-octane and its blends. Drawn in the background is the spark plug with its three electrodes for positional reference (intake valves at the top of each graph, exhaust valves at the bottom). The starting point of each

path is marked by a cross. The centroid end point was always naturally the cylinder bore's centre when the flame had occupied the whole piston crown window area. All fuels propagated towards the exhaust side with a note that both 25% ethanol blends (E25 and E25I75) had a clear tendency of centroid motion towards one side of the engine (positive z -direction), particularly at hot engine conditions, while the other fuels remained mostly closer to the central symmetry line. Gasoline at cold engine conditions for $\phi=0.83$ developed distinctively towards the negative z -direction, *i.e.* opposite to the general trend of E25. At cold conditions and irrespective of equivalence ratio, butanol always developed in the positive z -direction further than all the other fuels.

Considering that the y -axis was a symmetry axis of the mean in-cylinder flow field (**Figure 24**), any kernel drifting away from the centre-line moved further in that direction and part of the cylinder as the bulk flow was characterised by the presence of two counter-rotating vortices, each under one of the intake valves. Whether there was an effect of the type of fuel on the exact location of the spark's occurrence at the start of combustion remains unclear. Nevertheless, it is not immediately expected that spray differences between gasoline and E25 or E25I75 at hot engine conditions would lead to such strong bias towards the right of the spark plug for E25.

Stoichiometric fuelling featured a shorter path of centroid displacement towards the exhaust side of the engine. This is believed to be an effect of flow field at the later spark timing used for $\phi=1.0$ rather than sole contribution from the faster flame speed, as the v -velocity magnitude gradually decreased when approaching TDC (Malcolm *et al.*, 2011; Aleiferis *et al.*, 2016). Specifically, during the first 20° CA AIT for $\phi=0.83$ with spark advance of 36° CA, the v -velocity at ignition timing was predominantly 8–6 m/s in the direction from inlet to exhaust but it had clearly reduced to 2–4 m/s by 26° CA BTDC where the spark timing occurred for $\phi=1.0$.

The flame centroid's position recorded at each crank angle was used to quantify a measure of global motion velocity as the ratio of the displacement with respect to the initial centroid location at ignition timing to the overall time elapsed since the ignition. The average centroid v -velocity shown in **Figure 27** for the gasoline-based fuels and **Figure 28** for the *iso*-octane-based fuels, may be compared to the ensemble averaged air-flow velocity measured by LDV by Malcolm *et al.* (2011) and Aleiferis *et al.* (2016) that has been included in **Figures 27–28** as thick black dotted lines. For stoichiometric conditions, the flame centroid velocity clearly follows the air-flow velocity over the period 5–25° CA AIT, exhibiting continuously reducing magnitude (note the negative scale on the velocity axis) till the onset of flame clipping by the boundary of the piston's optical crown (25–35° CA AIT). From that point onwards, the airflow trace remains nearly constant but the magnitude of the flame centroid velocity reduces further while filling gradually the whole of the optical bore. At the later stages of combustion, as the flame centroid moves back towards the combustion chamber's central region, it returns slightly positive velocities.

The flame centroid velocity was higher in magnitude for stoichiometric conditions with their later spark timings, than for lean conditions. It is also interesting to note that the centroid velocities for $\phi=1$ remain typically below the 'horizon' of the airflow velocity trace in the region 5–25° CA AIT irrespective of engine temperature, whilst for $\phi=0.83$ they rest clearly above that horizon. This highlights that the lean flames were not 'convected' by the airflow as strongly as the stoichiometric flames.

At 20 °C engine temperature, all fuels showed similar development. Only lean butanol featured quite lower velocities than the other fuels at its coldest engine setting of 45 °C, but this agrees with its different behaviour as a whole at these conditions established earlier and possibly stemming from quite poorer atomisation. The differences between fuels increased at 80 °C engine temperature, more so at $\phi=0.83$ for the gasoline–alcohol mixtures.

COMBUSTION DIAGRAMS

Chemical and Turbulent Scales

Finalising the analysis of the combustion investigation and the comparison between the alcohols with *iso*-octane (gasoline was not evaluated separately due to lack of knowledge of all necessary properties), the burning regimes are shown using combustion diagrams for qualitative comparison. To do that it was necessary to estimate various combustion parameters as shown in **Table 7**. The laminar burning velocities of Broustail *et al.* (2011, 2013) at conditions of 5 bar, 423 K were used as baseline u_l , while all the other parameters were calculated for 5 bar, 500 K, the approximate pressure and temperature at the time of ignition. The laminar flame thickness δ_l was obtained by the ratio of the mass diffusion coefficient (averaged between rich and lean conditions) to the laminar burning velocity u_l , the chemical reaction time τ_l as the ratio of δ_l to u_l and the eddy turnover time τ_L as ratio of the integral length scale L to turbulence intensity u' . The turbulence intensity u' and integral length scale L were taken from PIV and LDV measurements in this engine (Malcolm *et al.*, 2011; Aleiferis *et al.*, 2016). The integral length scale in the vicinity of the spark plug was measured at about 5 mm by PIV (Aleiferis and Behringer, 2015). The choice of a suitable turbulence intensity posed some challenges. Using ensemble averaging, u' was measured at 3 m/s by PIV and LDV, but if one employed techniques to distinguish between large scale cyclic variations and high frequency fluctuations within cycles, u' returned values of about 1.5 m/s (Aleiferis *et al.*, 2016)

Thermophysical properties were taken from Yaws (2003). Then other turbulence characteristics were estimated by conventional relationships, namely the Kolmogorov length scale $l_k = Re_L^{-3/4}$, the dissipation rate $\varepsilon = u'^3/L$, the Kolmogorov time scale $\tau_k = (\nu/\varepsilon)^{1/2}$ and the Taylor length scale $l_T = (15\nu u'^2/\varepsilon)^{1/2}$. The Kolmogorov length scales were estimated at ~ 0.026 mm (where the kinetic energy is dissipated by the viscosity). The energy cascades down from integral to Kolmogorov scales, through the Taylor scale, estimated at ~ 0.6 mm for $u' = 1.5$ m/s. While the Taylor length scale has no clear structural definition, it could be seen as the distance that a Kolmogorov structure is transported by the larger eddies during its turnover time. For completeness it is noted though that Pope (1987) points out that the Kolmogorov scale underestimates the size of the smallest existing eddies by approximately an order of magnitude. It is also noted that in practice the smallest length scales that can influence the flame in engines are defined by the Gibson length $l_G = L(u'/u_l)^{-3}$ (Peters, 1986). That was estimated at ~ 0.1 mm for $u' = 1.5$ m/s.

The analysis led to Damköhler numbers between 70 and 90 for $u' = 1.5$ m/s. Larger Damköhler numbers signify fast combustion chemistry in comparison to the residence time in the turbulent flow, thus stabilising the combustion. The inverse of the Damköhler number returns the Karlovitz number, when using the Kolmogorov time scale instead of the integral time scale in the ratio with the chemical timescale. Small Karlovitz numbers indicate that the turbulence and related flame stretch is smaller than the chemical time, promoting stable combustion in the case of $Ka < 1$. The Lewis number calculation for lean and rich conditions was based on Abdel-Gayed *et al.* (1984a,b) with weighting applied for stoichiometric conditions. The turbulent Reynolds numbers found were between 1188–1212 and therefore just within 2% of each other, using $u' = 1.5$ m/s. If $u' = 3$ m/s was used, the Reynolds numbers would be double with values around 2400. The Karlovitz number would approximately triple and conversely, the effect on the Damköhler number would result in a reduction by approximately 40%, significantly affecting the location of the data points on the combustion diagrams. This highlights the importance (and ambiguity) of well-defined turbulence properties on the combustion analysis using such charts. Two turbulent Karlovitz stretch factors K are

also given in **Table 7** for completeness, calculated according to Bradley *et al.* (2000) as: $K_{(a)}=0.157(u'/u_l)^2 Re_L^{-1/2}$ or as used by Bradley *et al.* (2011a) with a constant of 0.250 instead of 0.157.

Abraham Combustion Diagram

When carrying the $\phi=1.0$ tabular values over into the Abraham plot in **Figure 29**, showing Da vs. Re_L , it can be seen that the three single component fuels, for both cases of turbulence intensities (circles correspond to $u'=1.5$ m/s, crosses to $u'=3$ m/s), rest in the yellow region which was drawn in the original paper by Abraham *et al.* (1985) to indicate a typical region associated with internal combustion engines. The Reynolds number of all fuels is similar, but the effect of the different u' becomes obvious, with the 3 m/s value having higher Re_L but lower Da . As a direct result, the fuels lay more towards the lower right corner of the yellow region which is normally associated with lower laminar burning speeds. The fuels are resting below the $l_k/\delta_l=1$ limit, *i.e.* between the reaction sheet and distributed reaction zones in an area of yet not too clear combustion characteristics, also known as intermediate regime between the regions of distributed and multiple flame sheets.

When changing to lean conditions of $\phi=0.83$ at identical turbulence, pressure and temperature conditions, using changing only the fuels' mass diffusion coefficient (as the fuel is now the deficient reactant) and using laminar flame speeds of 0.34 m/s for the alcohols and 0.3 m/s for *iso*-octane (Broustail *et al.*, 2013), Re_L values would remain identical but Da values would increase for *iso*-octane by 30% and for butanol by 8%, but would decrease for ethanol by 17%. Only when the in-cylinder conditions would be corrected to those at the earlier spark timing for used for $\phi=0.83$, a significant displacement towards the lower left would be seen (caused by Re_L reduction to ~ 1100 and Da to 45–66. All fuel points would however still rest within the yellow zone and within the reaction sheet region (not shown in the graph).

For $u' = 3.0$ m/s, the laminar flame time scale would be larger than the timescale of turbulent straining (Kolmogorov time scale) by about 30%. The flames wouldn't fulfil the conditions equivalent to the flame-sheet regime, namely $l_k/\delta_l < 1$ and $\tau_L < \tau_k$, and the flame would therefore not necessarily feature a thin flame sheet. Yet, as the conditions are borderline and not significantly undercut by any fuel, the occurrence of turbulent motion within the reaction area should not heavily affect the convective-diffusive balance in the preheat zone, but local extinction of the flame due to straining (τ_k smaller than τ_l) may occur (Pope, 1987). No distinct regions of flame extinction could be recognised from flame tomography imaging with the same base fuels in the current engine (Aleiferis and Behringer, 2015). The boundaries in the Abraham plot obviously do not correspond to absolute step changes but offer soft order-of-magnitude transition regions, so that even with $u'=3$ m/s the flame could still progress as a thin, single (or in multiple) sheet(s). In contrast, when $u'=1.5$ m/s is used (circles), the data points located more centrally in the yellow area and rest well within the boundaries of the reaction sheet region. The differences between the fuels are very small in both cases.

Peters Combustion Diagram

The Peters combustion diagram in **Figure 29** (Peters, 1986) shows the ratio of u'/u_l against the ratio of L/δ_l . The diagram displays regions for fast and slow combustion chemistry in relation to the ambient turbulence for $Da > 0$ and $Da < 0$, respectively, alongside regions of strong and weak flame stretch. Strongly stretched flames can be expected in areas of $Ka > 1$, while $Ka < 1$ signifies low stretch with a chemical time lower than the time scale of the smallest eddies – which therefore cannot significantly affect the reaction front and preheat regions and combustion remains quasi-steady.

When placed on this plot for $\phi=1.0$ the values for all three fuels generally confirm the conclusions taken from the Abraham plot, showing that for the lower u' case all fuels are located well within the corrugated flamelet region below the $Ka<1$ threshold, *i.e.* where the flame thickness is smaller than the Kolmogorov scale. All fuels appear again very close together, with the alcohols showing the same u'/u_l ratio but slightly differing positions along the horizontal axis due to the lower flame thickness δ_l calculated for butanol. In comparison, *iso*-Octane rests between the two alcohols in terms of δ_l but its lower u_l shifted its location on the chart to slightly higher values along the vertical axis. Using $\phi=0.83$ at identical in-cylinder conditions but with adjusted u_l and mass diffusion, all data points would be slightly shifted to the top right due to smaller δ_l and u_l . As for Abraham's plot, all three fuels would still be located in the corrugated flamelet region.

Using a higher turbulence intensity of $u'=3$ m/s, would suggest that the flames be slightly above the $Ka=1$ borderline and into the corrugated flames regime within the distributed reaction zone ($Ka=1.1-1.4$). Here, the chemical reaction in the flame front would be affected by the regnant turbulence in terms of the smallest eddies that may enter the reactive-diffusive flame structure in the preheat zone, but cannot enter the inner layer where the actual fuel consumption takes place and the layer is embedded within the quasi-laminar flow of the eddy. If the Kolmogorov eddies however became smaller than the inner layer, then the chemical reaction zone would be disturbed and the flame would likely extinguish locally ('broken reaction zone', located above the distributed reaction zone). However, for the prevailing conditions, the closeness to the regional boundary would suggest that the effect on the flame front is small. Also Peters in his modified diagram (Peters, 1999) commented that a line at $Ka=100$ (close to the boundary area identified by the DNS work of Poinso *et al.* (1990) as a new limit of an extended flamelet regime) can be used to define a new 'thickened wrinkled flame' or thin reaction zones' regime above $Ka=1$. This corresponds to a length-scale of the order the flame's inner layer thickness that is about 10% of the laminar flame thickness.

Leeds Combustion Diagram

For completeness the Leeds diagram as compiled by Bradley (1992) is included in **Figure 30**. The diagram highlights the effect of the Lewis number which is relating thermal and mass diffusion balance effects and gives an indication about the stability of the flame front in terms of different flame velocities in regions of positive (crests) and negative (cusps) stretch over the flame front. The horizontal axis on this diagram is built from a measure of wrinkling factor defined by the ratio of effective turbulence intensity u_k' to u_l (where u_k' can be exchanged by u' for fully developed turbulence). The vertical axis gives the ratio of turbulent to laminar burning velocities u_t/u_l . The diagram contains lines for constant products of KLe (solid lines), as well as constant ratios of Re_L to the square of Le (dashed lines). The combined consideration of K and Le for comparison is useful, as both numbers independently evaluate the flame stability and may have opposing or amplifying effects. Small K values indicate small stretch due to the chemical time being much faster than the time scale of turbulence (thus reducing the turbulence-induced stretch effect), while large Le values indicate stronger heat loss of the flame front compared to the reactant transport based on mass diffusivity (what would decrease the flame speed at positively stretched and increase them at negatively stretched regions, providing stability). Low values of KLe correspond with flames featuring a continuous wrinkled laminar flame sheet, while higher KLe values indicate a greater extent of fragmentation caused by increased flame stretch up to the point of quenching at the boundary condition of $KLe=5.3$ corresponding to the work of Poinso *et al.* (1990).

The positions of the fuel data in the chart were obtained by following the calculated KLe values until their intersection with the u'/u_i ratio. For the lower turbulence intensity of $u'=1.5$ m/s, the resulting locations showed KLe values of 0.07–0.09 for the alcohols and 0.15 for *iso*-octane, as well as horizontal axis values of 3.6 for the alcohols and 4.1 for *iso*-octane (shown in the chart by circular markers). Those values are consistent with the in-cylinder flame speeds discussed earlier. The values for the higher turbulence intensity of $u'=3$ m/s have also been included in the chart by square markers and rest generally towards higher KLe and u'/u_i values (both approximately doubled) when compared to u' of 1.5 m/s. Using $\phi=0.83$ at identical in-cylinder conditions but adjusted u_i and Le , all data points would be slightly towards higher values of KLe (approximately doubled) and higher u'/u_i values (approximately 20% higher).

It is important at this stage to close with a disclaimer, reminding that the use of such parameters and diagrams provides only a rough qualitative measure and requires cautious interpretation, while pointing out that these are the only possible means currently available to estimate the regimes of combustion. The ambiguity in the calculation of u' , as well as the true localised ϕ , temperature and residual gas fraction in real engines, would require more research work at heavily controlled conditions in constant volume vessels but also in a variety of optical engines for insights on a scale better than the order-of-magnitude valid resolution of those combustion diagrams.

In the context of DISI engines it is also of interest to understand the effect of mixtures that may still carry fuel droplets. For example, *iso*-octane aerosols in constant volume combustion vessels have shown that existence of micron-size droplets in the mixture field can affect burning rates significantly at laminar conditions but the effect is quickly negated by turbulence and can become insignificant at typical in-cylinder levels of turbulence intensity (Atzler *et al.*, 2006; Lawes and Saat, 2011); however, no data exist with lower volatility or higher latent heat fuels like butanol and ethanol, respectively.

SUMMARY AND CONCLUSIONS

The current article presented results from a series of engine experiments aimed at comparing the combustion behaviour of gasoline, *iso*-octane, ethanol, butanol, 25% blends of each of the two alcohols with gasoline (E25, B25) and with *iso*-octane (E25I75, B25I75), as well as 16% blends of butanol with gasoline (B16, equivalent in oxygen content to E10) and with *iso*-octane (B16I84). The engine was run at 1500 RPM, 0.5 bar intake pressure with stoichiometric and lean mixtures ($\phi=1.0$ and $\phi=0.83$) prepared by direct fuel injection during the early intake stroke for ‘homogeneous’ operation. The MBT spark timing was identified for each fuel at 80 °C engine coolant temperature. Flame chemiluminescence imaging was performed with one crank-angle resolution for a series of consecutive cycles using colour and monochrome cameras at the MBT spark advance of gasoline for all fuels (selected to fix in-cylinder pressure, temperature and flow at the onset of combustion for all fuels). The greyscale flame images were post-processed to infer rates of flame growth and in-cylinder motion at cold and hot engine conditions. The main conclusions of this study can be summarised as follows:

Thermodynamic Analysis

- When comparing fuels at their own MBT spark advance, at $\phi=1.0$, ethanol returned the highest IMEP, ~3% above gasoline’s despite its lower absolute (per kg fuel) and relative (per kg air of the mixture) heating value. At $\phi=0.83$, no major difference was observed between ethanol’s and gasoline’s IMEP. Butanol, despite having the largest relative (per kg air) energy content, exhibited an IMEP about 7% lower than ethanol’s and 4% lower than gasoline’s at $\phi=1.0$. At $\phi=0.83$, butanol showed about 5% lower IMEP than ethanol.

- The COV_{IMEP} of all fuels was generally below 2% at their fuel-specific MBT spark timings, with the exception of lean *iso*-octane which showed elevated levels to about 4–5% and with audible combustion instability and misfire when moved away from its MBT spark timing.

Flame Chemiluminescence Imaging

- The flames of both gasoline and *iso*-octane were blue in colour, with *iso*-octane exhibiting lower luminosity than all the other fuels, especially for lean conditions. Ethanol and butanol were both featuring an orange-yellow flame centre, which could be considered to stem from broadband incandescence of burning droplets. However, this effect should have been stronger for butanol that featured distinctly larger droplets during injection than all fuels, but it was ethanol showing this colouring feature more distinctly. It may be that any remaining of butanol's larger droplets at ignition timing were more dispersed and lower in number compared to ethanol, or that ethanol suffered from slower evaporation rates past injection due to latent heat effects.
- Flame imaging for cold butanol was not possible at 20 °C engine coolant temperature and required 35 °C when stoichiometric and 45 °C when lean to achieve relatively stable combustion. This is believed to originate from poor fuel atomisation at cold engine conditions due to butanol's distinctly larger viscosity than that of the other fuels. Higher injection pressures could bring some improvement, but higher penetration and successive piston impingement could follow, therefore more advanced injection strategies with multiple 'split' injection events would be beneficial. The butanol blends did not show any issues with combustion stability at 20 °C.
- Image processing showed that the hydrocarbon fuels and their alcohol blends exhibited initial combustion delay that was increasing at lower engine temperature or lean conditions. The pure alcohols were relatively insensitive to changes in temperature at $\phi=1.0$, but did show an increased initial combustion delay for cold engine at $\phi=0.83$.
- Ethanol's early flame growth rate was distinctly the fastest throughout.
- The early flame development of gasoline was faster than *iso*-octane's at all but hot-engine lean conditions. This observation was not in absolute agreement with the thermodynamic results, where gasoline was always faster than *iso*-octane to 10% MFB, even at $\phi=0.83$, 80 °C.
- Butanol showed faster flame growth rate than gasoline at lean conditions but similar when stoichiometric. Butanol's flame area showed the largest standard deviation (20–25% of the mean), highlighting its high combustion variability. Ethanol showed the lowest variability throughout with levels as low as 5–10% at hot stoichiometric engine conditions.
- Lean flame speeds were typically 20–30% lower than for stoichiometric conditions depending on fuel type.
- The peak flame growth speeds were found to be for 19% higher for ethanol than for *iso*-octane at stoichiometric conditions; this correlates with the 17% difference found for the laminar flame speeds of the two fuels by Broustail *et al.* (2013) at 5 bar 423 K. However, the latter authors reported similar values for butanol and ethanol, although in the engine butanol was faster than *iso*-octane by about 7%.
- E25 progressed generally between the constituents at $\phi=1$, hot-engine conditions. At hot lean conditions though it exhibited benefits as its flame speed was distinctly higher than gasoline's, reaching the levels of ethanol.
- The *iso*-octane–alcohol blends showed flame growth speeds closer to *iso*-octane's. E25I75 had slightly lower speed than *iso*-octane at $\phi=0.83$, with the trend inversed at $\phi=1.0$. Cold engine conditions were associated with a decrease in B25I75's flame speed; this suggests a blending limit in terms of combustion stability. B25 did not

show this behaviour. Otherwise, all butanol blends exhibited faster burning than *iso*-octane. These trends were in general agreement with the laminar flame speeds of Broustail *et al.* (2013) at 423 K, 1 bar, where the alcohol blends exhibited speeds slightly above *iso*-octane's at $\phi=1.0$ and reduced flame speed for E25I75 at $\phi=0.8$.

- For $\phi=1.0$ the flame stretch rate reduced from levels of 3–6 ms⁻¹ at flame radii of 2 mm to about 2 ms⁻¹ at 10 mm. There were small differences among fuels; ethanol exhibited generally the highest levels, *iso*-octane the lowest and butanol in-between. The separation between fuels was clearer at 20 °C than at 80 °C and early stretch rates higher; ethanol showed higher initial stretch at 80 °C though. Lower levels of stretch were recorded for $\phi=0.83$, with initial levels at radii of 2–3 mm lower than 3 ms⁻¹.
- Ethanol's fastest flame growth speed may be related not only to its high laminar burning velocity but also to the lower Lewis number calculated for ethanol, maintaining the speed of combustion at high flame stretch at small flame radii more than other fuels. At lean conditions, where the Lewis number was far above unity for all fuels, ethanol's early flame development was more similar to the other fuels.
- The flame roundness showed a maximum value of ~30% at flame radii of ~2 mm, successively reducing and attaining levels of ~20–25% at flame radii of 10 mm for stoichiometric and 10–15% for lean conditions.
- The flame centroid motion path was found to follow the in-cylinder mean airflow pattern measured by PIV, depending on the side of spark appearance. Effects of local fuel concentration and temperature cannot be excluded as differences between fuels were observed despite their following the mean direction of in-cylinder motion. $\phi=1.0$ was associated with flame centroid velocities equal to or higher (in absolute terms) than the airflow velocity measured by LDV. $\phi=0.83$ exhibited lower or equal flame centroid velocities to the airflow.

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APPENDIX

A1. PRESSURE TRACES ACQUIRED AT FLAME IMAGING SPARK CONDITIONS

A2. MFB FROM FLAME IMAGING AND THERMODYNAMIC ANALYSIS

A comparison of the early MFB obtained from imaging and thermodynamic analysis shows the limitations of the pressure-based analysis to resolve the early flame development. It also highlights effects related to thermodynamic analysis of pressure signals from a research engine under optical and non-optical configuration. A common early crank angle was selected for which even the fastest fuel's radius was not exceeding the optical boundaries of the piston crown, but was late enough to identify calculated heat release effects from the in-cylinder pressure records, to compare at the same crank angle after ignition timing. The flame area analysis showed flame radii between 4–14 mm for 18° CA AIT at $\phi=1.0$ and 25° CA AIT at $\phi=0.83$ for all fuels, with ethanol flames being just about on the verge of getting clipped by the piston's optical boundary, so these crank angles were finally used for this exercise.

To estimate MFB from imaging, the burned gas volume was calculated from the flame radius by $V_b=4/3r^3\pi$ and weighted to mass by the burned gas density ρ_b . The ratio between unburned to burned gas density is approximately constant throughout the combustion and close to a value of 4 and the mass fraction burned x_b can be calculated according to Beretta *et al.* (1983). The gas densities were obtained by Morley (2005) for the in-cylinder conditions at stoichiometric spark timing (4.8 bar, 550 K) and a ratio of $\rho_u/\rho_b=4.7$ was calculated. Lean conditions at the respective spark timing conditions (3.5 bar, 500 K) returned an almost identical density ratio. The density ratio was also checked against the method of Andrews and Bradley (1972a,b), based on the ratio of unburned to burned gas

temperatures T_u/T_b corrected by the mole fraction of products to reactants and a flame thickness adjustment factor. Considering the similar starting pressures and temperatures for all fuels and the very similar adiabatic flame temperatures (Hara and Tanoue, 2006; Wu and Law, 2013), this ratio is expected to change only slightly within the range of the current fuels. Using a ratio of 4.7 for a flame radius of 14 mm, the respective MFB was ~6%.

Full comparison between the MFB results derived from the thermodynamic mapping work of the engine in full metal configuration, the MFB estimated from the images and the respective MFB results from the thermodynamic analysis results of in-cylinder pressure traces of the engine in optical configuration are presented in **Figure A2.1** for both $\phi=1$ and $\phi=0.83$. The differences in MFB obtained from imaging and thermodynamic analysis at such early crank angles was quite large in relative terms, but was usually within an absolute MFB of 1%, with the exception of ethanol which returned significantly higher MFB results for the optical investigation. For ethanol this may likely be an effect of the overestimation of the burned gas volume due to the relatively large size of the flame diameter at this specific timing (14 mm). The results also demonstrate significant differences between the heat release analysis of the pressure signals from the non-optical engine configuration with its long stabilisation time and the tests with optical access with its limited firing time, what would typically result in larger heat losses. For the optical configuration, the pressure-based MFB results were very low, at cases not recording values greater than zero. This also highlights issues between different engines in the literature when it comes to comparisons with other published data for truly engine-independent quantitative conclusions.

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NOMENCLATURE

Da	Damköhler number
δ_l	Laminar flame thickness
ε	Dissipation rate
K	Karlovitz stretch factor
Ka	Karlovitz number
L	Integral length scale
l_G	Gibson length scale
l_k	Kolmogorov length scale
l_T	Taylor length scale
Le	Lewis number
λ	Air excess ratio
Ma	Markstein number
ν	Kinematic viscosity
P	Pressure
Re_L	Reynolds number with respect to integral length scale
ρ	Density
T	Temperature
τ_k	Kolmogorov timescale
τ_l	Timescale of laminar burning
τ_L	Eddy turnover time
u'	Turbulence intensity
u_k'	Effective turbulence intensity
u_l	Laminar burning velocity
x, y, z	Co-ordinates
ϕ	Equivalence ratio

ABBREVIATIONS

AIT	After Ignition Timing
ATDC	After intake Top Dead Centre
BTDC	Before compression Top Dead Centre
CA	Crank Angle
COV	Coefficient Of Variation
DISI	Direct Injection Spark Ignition
EVC	Exhaust Valve Closure
EVO	Exhaust Valve Open
IMEP	Indicated Mean Effective Pressure
IVC	Intake Valve Closure
IVO	Intake Valve Open
LDV	Laser Doppler Velocimetry
MBT	Minimum spark advance for Best Torque
MFB	Mass Fraction Burned
PFI	Port Fuel Injection
PIV	Particle Image Velocimetry
RPM	Revolutions Per Minute
SI	Spark Ignition
SMD	Sauter Mean Diameter

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Table 1. Properties of base fuels.

Fuel	Ethanol	Butanol	Gasoline	<i>iso</i> -Octane
Chemical formula	C ₂ H ₅ OH	C ₄ H ₉ OH	~C ₄ –C ₁₂	C ₈ H ₁₈
Molar mass [g/mol]	46.07	74.12	100–105	114.3
Density, 20 °C, 80 °C [g/cm ³]	0.79, 0.73	0.81, 0.76	0.72, 0.66	0.69, 0.64
Solubility in water (20 °C) [g/l]	miscible	79	partially	immiscible
DVPE, 20 °C [kPa]	6.4	0.8	35	5.7
DVPE, 37.8 °C (~RVP) [kPa]	16.1	2.2	72.4	11.8
DVPE, 80 °C [kPa]	100	16.4	208	50
Bubble Point (0.5 bar) [°C]	62.6	108.8	29.8	80
Kinematic viscosity (23 °C) [cSt]	1.33	3.22	0.47	0.62
Kinematic viscosity (80 °C) [cSt]	0.60	0.99	0.25	0.40
Surface tension (23 °C) [mN/m]	23.01	25.50	21.80	18.78
Surface tension (80 °C) [mN/m]	16.4	19.3	–	13.6
Latent heat, 25 °C [kJ/kg]	874	669	380–500	300
Latent heat (at boiling) [kJ/kg]	855	584	364	272
Specific heat, 25 °C [kJ/kgK]	2.46	2.30	2.22	2.09
Explosion limit (upper) [Vol%]	15	11.3	7.6	6
Explosion limit (lower) [Vol%]	3.5	1.4	1.4	1
Stoichiometric AFR	9	11.1	14.6	15.1
Heating value [MJ/kg], [MJ/l]	26.9, 21.3	33.9, 27.5	42.7, 32	44.6, 30.8
RON	129	96	95	100
H/C, O/C	3, 0.5	2.5, 0.25	1.92, 0	2.25, 0

Table 2. Properties of blends.

Fuel	E25	E25I75	B16	B25	B16I84	B25I75
Molar mass [g/mol]	78	81	96	93	104	99
Density, 20 °C, 80 °C [g/cm ³]	0.76	0.71	0.75	0.75	0.70	0.72
Density, 80 °C [g/cm ³]	0.68	0.66	0.70	0.70	0.65	0.67
DVPE, 20 °C [kPa]	38	11	32	30	8	8
DVPE, 37.8 °C (~RVP) [kPa]	73.8	26.5	66.3	62.9	14.7	14.4
DVPE, 80 °C [kPa]	240	140	194	188	70	69
Kinematic viscosity, 20 °C [cSt]	0.75	0.89	0.68	0.79	0.83	1.00
Kinematic viscosity, 80 °C [cSt]	0.37	0.58	0.34	0.39	0.54	0.55
Surface tension, 23 °C [mN/m]	21.5	19.3	21.0	21.5	18.7	18.8
Latent heat, 25 °C [kJ/kg]	491	433	401	422	329	360
Specific heat, 25 °C [kJ/kgK]	2.28	2.18	2.23	2.28	2.12	2.14
Stoichiometric AFR	13.0	13.4	14.0	13.6	14.2	13.9

Table 3. Laminar flame speed of ethanol and butanol and their blends in gasoline.

T [K]	P [bar]	ϕ [–]	Gasoline [cm/s]	E25 [cm/s]	E50 [cm/s]	E75 [cm/s]	Ethanol [cm/s]
358–373	5	1	31.0	31.0	31.0	31.0	31.0
358–373	10	1	28	28.1	28.3	28.4	27.5
358–373	5	0.8	22.0	22.0	22.0	22.0	22.0
358–373	10	0.8	19	19.4	19.8	20.2	17.5

T [K]	P [bar]	ϕ [–]	Gasoline [cm/s]	B25 [cm/s]	B50 [cm/s]	B75 [cm/s]	Butanol [cm/s]
358–373	5	1	31.0	30.8	30.5	30.3	32.0
358–373	10	1	28.0	28.0	28.0	28.0	28.0
358–373	5	0.8	22.0	22.0	22.0	22.0	22.0
358–373	10	0.8	19.0	19.3	19.5	19.8	18.0

Table 4. Laminar flame speed of ethanol and butanol and their blends in *iso*-octane.

T [K]	P [bar]	ϕ [–]	<i>iso</i>-Octane [cm/s]	E25I75 [cm/s]	E50I50 [cm/s]	E75I25 [cm/s]	Ethanol [cm/s]
393	1	1	51	52.5	57	59	63
358–373	5	1	30.0	29.8	29.5	29.3	31.0
358–373	10	1	27.0	26.9	26.8	26.6	27.5
393	1	0.8	38	39	43	46	48
358–373	5	0.8	21.0	20.8	20.5	20.3	22.0
358–373	10	0.8	17.0	16.9	16.8	16.6	17.5

T [K]	P [bar]	ϕ [–]	<i>iso</i>-Octane [cm/s]	B25I75 [cm/s]	B50I50 [cm/s]	B75I25 [cm/s]	Butanol [cm/s]
393	1	1	51	51	52.5	56	58
358–373	5	1	30.0	29.5	29.0	28.6	32.0
358–373	10	1	27.0	26.8	26.5	26.3	28.0
393	1	0.8	38	38	39.5	40	46
358–373	5	0.8	21.0	20.8	20.5	20.3	22.0
358–373	10	0.8	17.0	16.8	16.5	16.3	18.0

Table 5. Engine specifications.

Engine Parameter	Value
Bore [mm] $\times$ Stroke [mm]	82.5 $\times$ 88.9
Displacement [cm ³]	475
Compression Ratio	9.8:1
Number of Valves	2 Inlet, 2 Exhaust
Inlet Valve Opening, Closing	349.5° CA, -124.5° CA ATDC Compression
Exhaust Valve Opening, Closing	118° CA, -359° CA ATDC Compression

Table 6. MBT spark advance for all fuels.

Fuel	MBT, $\phi=1.0$ [°CA BTDC]	MBT, $\phi=0.83$ [°CA BTDC]
Gasoline	26	36
<i>iso</i> -Octane	29	45
Ethanol	25	32
Butanol	25	34
B16	25	35
B25	25	35
E25	25	35
B16I84	29	40
B25I75	27	38
E25I75	28	41

Table 7. Estimated turbulence and combustion parameters for the single-component fuels.

Parameter	<i>iso</i> -Octane	Ethanol	Butanol
Laminar Flame Speed, u_l [m/s]	0.36	0.42	0.42
Laminar Flame Thickness, δ_l [mm]	0.0185	0.0193	0.017
Chemical Reaction Timescale, τ_l [ms]	0.052	0.046	0.041
Kolmogorov Lengthscale, l_k [mm]	0.027	0.027	0.026
Kolmogorov Timescale, τ_k [ms]	0.106	0.106	0.105
Taylor Lengthscale, l_T [mm]	0.65	0.64	0.61
Turbulent Reynolds Number, Re_L [-]	1189	1197	1212
Lewis Number (Lean, Rich), Le [-]	0.92, 2.79	0.92, 1.50	0.91, 2.12
Damköhler Number, Da [-]	71.1	79.7	90.0
Kalovitz Number, Ka [-]	0.48	0.43	0.39
Karlovitz Stretch Factor, $K_{(a)}$, $K_{(b)}$ [-]	0.079, 0.126	0.058, 0.092	0.057, 0.091

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