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Spray and Combustion Characterization of the Alcohol Blends in the High-Pressure High-Temperature Conditions

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1. Introduction

In the last decades, compression-ignition (CI) engine has been strongly improved to meet higher stringent emissions regulations, especially in NO_x and Soot. At the same time, increasing concerns of the depletion of oil resources and the global warming by greenhouse effect gas, mainly by CO₂, lead to several alcohol fuels such as ethanol and butanol have been considered as an alternative fuel and renewable resources [1], [2]. Researchers consider low proportion of alcohol fuels as one mean to improve combustion efficiency and to reduce NO_x and Soot emissions due to longer ignition delay, especially in advanced CI engine, based on Low Temperature Combustion [1]. On the other hand, the intermediate fermentation mixture of butanol production, called ABE (Acetone, Butanol and Ethanol), is more and more considered as one new alternative fuel for CI engine due to its physical and chemical properties, quite similar to butanol and the advantages of no over cost and energy consumption due to the separate process of butanol [3].

This paper presents the spray and combustion characterization on the currently interested alcohol fuels and ABE, blended with n-Dodecane in proportional 20% by volume, such as 20% v of butanol (Bu20), 20% v of ethanol (Eth20), and 20% v of Acetone-Butanol-Ethanol (ABE20). To discuss the effect of fuel, the results are compared with pure n-Dodecane (n-Do100) as the surrogate diesel fuel. The physical properties of the testing fuels are shown in Table 1.

The High-Pressure and High-Temperature (HPHT) chamber, called "New One Shot Engine" (NOSE), has been used to investigate the macroscopic spray and combustion parameters by validating Spray-A conditions, defined by Engine Combustion Network (<http://public.ca.sandia.gov/ecn>). Both non-reactive conditions (pure Nitrogen) and reactive conditions (15%

oxygen) were carried on the ambient pressure (near 60 bar), ambient density (22.8 kg/m³) and various ambient temperatures (800, 850, and 900 K). The main testing conditions are summarized in Table 2. Further details about the chamber design, thermal characterization chamber, specification of the injection system, and data acquisition system can be found in previous study [4].

Table. 1. Fuel properties.

Properties	n-Do100	ABE20	Bu20	Eth20
Molecular formula	C ₁₂ H ₂₆	C _{8.5} H _{18.6} O _{0.4} ^a	C _{8.9} H _{19.9} O _{0.4} ^a	C _{7.1} H _{16.1} O _{0.5} ^a
Density at 15 °C (kg/m ³)	752.8	760.7	763.3	758.8
Viscosity at 15 °C (mm ² /s)	2.032	1.642	2.124	1.881
Cetane number [5]	74	-	-	-
Boiling point (K) [6]	489	464 ^b	468 ^b	460 ^b
Vapor pressure at 298 K (kPa) [6]	0.02	2.17 ^b	0.14 ^b	1.66 ^b
Latent heat of Vaporization at 298 K (kJ/kg) [6], [7]	362	411 ^b	409 ^b	520 ^b
Oxygen Concentration (% by mass)	-	5.2%	4.6%	7.3%

Note: ^aThese formulas were calculated by mole fraction based on 1 mole of fuel.

^bThese properties were estimated by the mass fraction of single-component fuels in the alcohol blend.

Table. 2. Summary of testing condition.

Parameters	Value
Ambient gas temperature	800, 850, 900 K
Ambient gas pressure	near 60 bar
Ambient gas density	22.8 kg/m ³
Ambient gas oxygen	0% O ₂ for non-reactive 15% O ₂ for reactive
Fuel injection pressure	150 MPa (1,500 bar)
Fuel temperature at nozzle	363 K (90°C)
Injection duration	1.5 ms
Number of repetitive test	12 tests per condition

2. Optical Techniques

In this part, the optical setups for non-reactive and reactive conditions are briefly summarized. For more information are provided in previous works [3], [4].

2.1 Non-Reactive Condition

The liquid phase of spray has been characterized by the Diffused-Black Illumination (DBI) technique due to the easy implementation with LED light source and High speed camera, as shown in Fig. 1. For the post-processing, the average light intensity (I_{avg}) of the averaged image was normalized by background images (I_{bg}), obtained from the average of images before Start of Injection (SOI). The images during the steady state of injection, i.e. 1.1 to 1.5 ms after SOI, are also averaged to avoid the transient phases due to the start and end of injection. Then the light extinction factor, $\tau(x, y) = -\log\left(\frac{I_{avg}(x, y)}{I_{bg}(x, y)}\right)$, along the spray core was calculated. To avoid the effect of the beam steering phenomenon due to variation in the refraction index on the medium at the liquid spray tip, the distance where the linear fit line crosses the X-axis was determined as the liquid length (LL) of spray penetration as shown in Fig. 2. (left) [3].

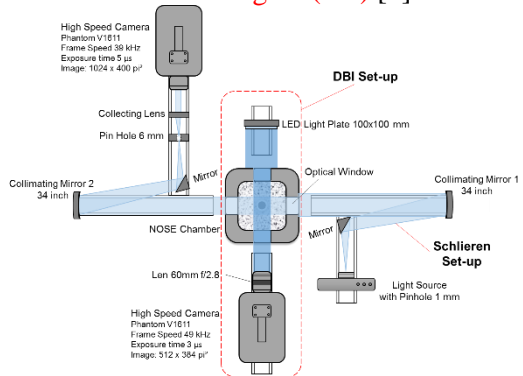


Fig. 1. Scheme of optical set-up for non-reactive condition.

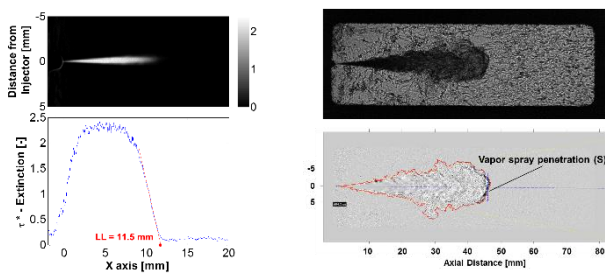


Fig. 2. The light extinction image (left-top), and criterion of LL determination (left-bottom). An example image of Schlieren (right-top) and an example post-processing to estimate S (right-bottom).

The vapor spray penetration (S) can be detected by the high-sensitivity of Schlieren technique. Based on the measurement of the deviation bending of the light source through the test section, which is sensitive enough to capture the vapor spray boundary. The

pinhole (or aperture) Schlieren stop was used to provide strong gradient between give a bright field and dark background as shown in Fig. 1. The standardized post-processing code of Sandia (<http://public.ca.sandia.gov/ecn>) was used to determinate S and also reduce uncertainties. An example of Schlieren image and the criterion to estimate S are illustrated in Fig. 2 (right).

2.2 Reactive Condition

Lift-Off Length (LOL) was defined as the distance between the injector tip and the stabilized flame of the high-temperature reaction zone [8]. At high temperature, the chemiluminescence spectrum of OH* is centered at 310 nm, so OH* is a good indicator to measure the LOL. As shown in Figure 3, an ICCD was used with a 60 mm f/3.5 UV lens and equipped with a 310 nm (FWHM10) band-pass filter (BFP). A long constant gating time of 449 μs was used to avoid effect of turbulent fluctuation in the LOL determination in order to provide an image of the ‘quasi-steady’ mean LOL after SOI [8]. The post-processing criterion to define LOL was the distance between the injector tip and the first value above 50% of the maximum intensity of the profile cross to the flame lope [9], as shown in Fig. 4. (left).

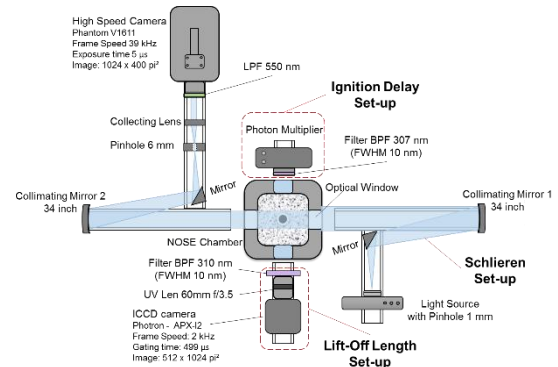


Fig. 3. Scheme of optical set-up for reactive condition.

Ignition Delay (ID) was defined as the time between the start of injection and the second stage of ignition, usually called the “main flame”. To detect the main flame ignition delay, a Photomultiplier tube side-on with a high voltage power supply and a band-pass filter of 307 nm (FWHM 10) was used to follow the temporal OH* chemiluminescence, as shown in Fig. 3. The low light intensity signal from the combustion event was multiplied and recorded in an in-house Labview data acquisition system during an interval recording of 4 μs. The time at the start of combustion of the main flame ID is defined at the maximum of the first peak of the signal, which corrected by the hydraulic delay (HD) to provide the absolute ID. The HD was defined as the time between the current signal for the start of injection and the first injection image of the spray obtained by Schlieren visualization in each test. Fig. 4. (right) presents the

criterion of ID determination.

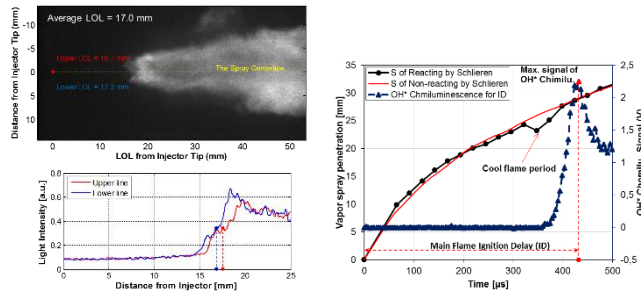


Fig. 4. An example of LOL result at 850 K of n-Do100 (left-top) and the criterion of LOL determination (left-bottom). The ID criterion of the OH* chemiluminescence signal is collected by a Photomultiplier at 900 K on n-Do100 (right).

3. Result and Discussion

3.1 Liquid Length (LL)

The effect of the ambient temperature of different fuel blends on LL is shown in Fig. 5. As well known, the higher energy entrainment due to higher ambient temperature increases the evaporation rate, leads to shorter LL. This trend is confirmed by Naber and Siebers’s Scaling law model [10] which is also plotted in Fig. 5. The ABE20 has the shortest LL for all ambient temperature, while the longest LL is obtained for Eth20. The shortest LL of ABE20 is mainly due to the higher volatility of the acetone in ABE20 [3] and also relate to Siebers’s work [11], concluded that the LL of a multi-component fuel is controlled by the component who provides the lower volatility. In the case of butanol or ethanol blends, the LL values are ranked as the latent heat of vaporization (LHV) values: from Bu20 to Eth20. The increase of the LHV induces a local cooling effect which may decrease the local ambient gas temperature and therefore reduce the rate of vaporization.

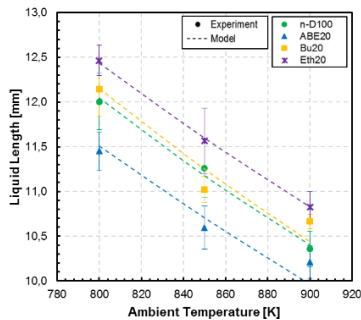


Fig. 5. The comparative result between the experimental results and Scaling law model for liquid length.

3.2 Vapor Spray Penetration (S)

Fig. 6 (left) shows the temporal evolution of S of ABE20 and Bu20 results after SOI in 3 various ambient temperatures. As the result, the difference for the ambient temperatures is slight as indicated low

standard deviation from the average of the three evolutions, as shown in Fig. 6 (left), the averaged STDs for all fuels are lower than 3%. For this reason, the averaged S of 3 ambient temperatures for all fuels was plotted in Fig. 6 (right). The result shows there is slightly different S in different fuel because of the small difference its fuel density. Indeed, S mainly depends on the spray momentum, which is controlled by the injection pressure (1500 bar), the ambient gas density (22.8 kg/m³), and the fuel density. From this hypothesis can be confirmed by the Musculus and Kattke’s model [12], which varied only the fuel density and kept the same other parameters for all fuels. Fig. 6 (right) plotted the simulation result of ABE20 and Bu20 and performed a good agreement with this expectation.

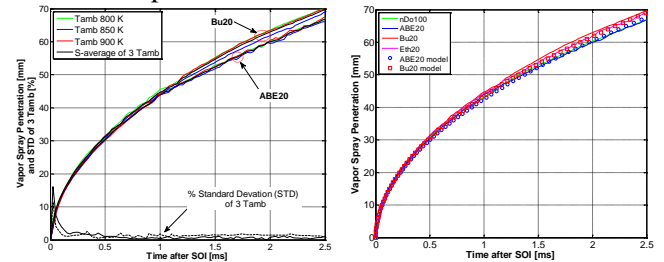


Fig. 6. Vapor spray penetration of ABE20 and Bu20 of 3 ambient temperatures (left) and the averaged vapor spray penetration of 3 ambient temperatures for all test fuels (right).

3.3 Lift-Off Length (LOL)

As expected, an increase of ambient temperature results in a faster local flame reaction rate, allowing the flame to stabilize closer to the injector and then decrease the LOL, as shown in Fig. 7 (left). The dot-lines represent the simulated results of the power-law empirical model, developed by Sieber and coworkers [8], [13], the results show the global agreement between the comparative result of the experimental results and simulation. The LOL as function of the alcohol blends can be ranked from shortest to longest as: n-Do100, ABE20, Bu20, and Eth20. Indeed, as LHV of all alcohol blends are higher than n-Do100, a longer LOL and ID are expected, due to the cooling effect of the chamber atmosphere and the increase of the vaporization time. But, in the case of ABE20, only slight difference to n-Do100 can be noticed for all ambient conditions. This could be explained by the fastest evaporation rate of ABE20 which is enhanced combustion by the mixing and evaporation process at upstream of LOL due to high volatility of acetone [3]. Also, as ABE has the blending ratio 3:6:1, LHV is lower than Ethanol, the impact of the cooling effect is less than other alcohol fuel.

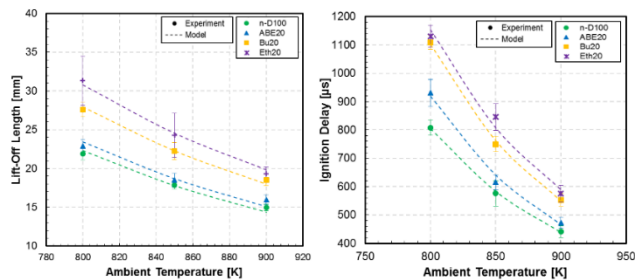


Fig. 7. Comparative result between experiment and simulation data of Lift-Off Length (left) and Ignition Delay (right) for all test fuels of 3 ambient temperatures.

3.4 Ignition Delay (ID)

Fig. 7 (right) shows the ID for all fuels decreases with the increase of the ambient temperature due to the lower fuel atomization and evaporation rate at lower ambient temperature, which is lower the chemical reaction rate [14]. The accuracy of the experimental results are validated by the trend of the Pickett and coworker's correlation [15], which globally matches very well with data. ID of n-Do100 is shorter than of alcohol blends due to the highest Cetane Number (74 for the n-Do100, while 8 and 17 for pure ethanol and butanol [5], respectively). For the alcohol blends, Eth20 is slightly longer ID than Bu20 as slightly higher CN of ethanol than butanol. But ID for ABE20 is closest to value of n-Do100 for the 3 ambient temperature and lower than other alcohol blends, as also for LOL.

4. Conclusion

The objective of this work was to characterize the behavior in spray and combustion of ABE20% – ndodecane80% mixture in the referenced conditions of ECN-Spray A. For that, a comparison with pure n-dodecane and ethanol or butanol blends was performed. The main results can be summarized as follows:

- There is no significant difference of the penetration length as function of different ambient temperatures for all blends, due to the slight difference of fuel density.
- The LHV and lower CN of Bu20 and Eth20 induce longer the LOL and ID than n-Do100.
- Due to high volatility, which favors the vaporization, ABE20 presents shorter LL than other alcohol blends and n-Do100. LOL and ID are in a good agreement with n-Do100 for the 3 ambient temperatures which confirms the high possibility of using ABE as substitute of diesel fuel.

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