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Spray and combustion characterizations of ABE/Dodecane blend in comparison to alcohol/Dodecane blends at high-pressure and high-temperature conditions

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ABSTRACT

This paper presents the spray and combustion characterization of Acetone-Butanol-Ethanol mixture and alcohol fuels, blended with n-Dodecane at different volume ratio, as 20% Acetone-Butanol-Ethanol (ABE20), 20% Butanol (Bu20), 40% Butanol (Bu40), 20% Ethanol (Eth20), as well as 20% Butanol/20% Ethanol (Bu20Eth20) to evaluate the impact of the physical and chemical characteristics, especially fuel oxygen contents. The experiments were carried out in "New One Shot Engine" at high-pressure and high-temperature conditions, established as Spray A condition, defined by Engine Combustion Network (ECN): 60 bar ambient pressure, 22.8 kg/m^3 ambient density and various ambient temperatures (800, 850, and 900 K). The liquid and vapor spray parameters were characterized by diffused-back illumination and Schlieren techniques in non-reactive condition (in pure nitrogen). In reactive conditions (with 15% oxygen), the lift-off length and absolute ignition delay were measured by OH* chemiluminescence.

First, as expected because of slight difference in fuel density, mass flow rates, vapor spray penetration, and spray angle are almost similar. But, due to the highest volatility, the liquid length of ABE20 is shorter compared to pure n-Dodecane and other blends. Also its ignition delay and lift-off length are shorter than those of alcohol blends due to difference in expected cetane number and latent heat of vaporization. The increase of butanol quantity or the addition of ethanol in blends increase the liquid length due to the cooling effect from the latent heat of vaporization, while the lift-off length and ignition delay increase with oxygen contents. Finally, ABE20 seems to be a good candidate for diesel-blended fuel due to the similar behavior as n-Dodecane itself.

1. Introduction

In the last decades, Compression-Ignition (CI) engines were strongly improved to respect more and more stringent emissions regulations, especially for NOx and Soot [1,2]. At the same time, increasing concerns of the depletion of oil resources and the global warming by greenhouse effect gases, mainly by CO2, the researchers search for alternative fuels to substitute the petroleum oil, as alcohol, biodiesel and biogas. However, substitute new fuels have to consider by following different steps of combustion process e.g. mixing formation, ignition and pollutant emissions. The mixing formation of diesel spray is an extensive research topic since the last two decades to improve the combustion efficiency and reduce the pollutant emissions. Macroscopic parameters such as liquid length penetration, vapor spray penetration and spreading spray angle, are the primary parameters to control the mixing formation [3]. Indeed, the liquid length penetration (LL) is one important parameter to design and optimize the operation of modern diesel engine, especially small-bore Direct-Injection diesel engine, to avoid impinges on piston bowl or cylinder walls, cause of high emissions [4]. LL can be shortened by decreasing the orifice diameter or/and increasing the ambient density or temperature. But no significant effect of the injection pressure was founded in the range of 40 to 160 MPa, while lower fuel volatility and fuel temperature provide longer LL [4]. The vapor phase penetration (S) and spray angle (θ) are 'indirect' parameters to qualify the fuel–air mixing process, strongly affected by the injector geometrical characteristics, spray momentum, gas density and fuel density [3,5,6].

To study Diesel combustion process itself, the Ignition Delay (ID) and Lift-off Length (LOL) of the flame are necessary parameters. ID represents the ability of fuels to auto-ignite, usually represented by the Cetane Number (CN): the highest CN corresponds to the shortest ID. The suitable value of ID depends of combustion mode: in Conventional

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Diesel Combustion, shorter ID (or higher CN) is favoured for smoother running. In the case of advanced combustion modes (as Low Temperature Combustion, Premixed Charge Compression Ignition or Homogeneous Charge Compression Ignition), the longer ID is required to reduce local equivalence ratio for soot formation reduction [7,8]. LOL represents the distance at which the entrained air, premixed with vaporized fuel is transported to the initial combustion zone downstream, so the distance from the injector tip to the reaction zone where the flame is stabilized. LOL depends on the ambient gases and injection conditions, and fuel properties. Moreover, fuels with shorter ID generally produce shorter LOL [7–10].

Some alcohol fuels, as ethanol, methanol, and butanol have been considered as alternative fuel for CI engines for the last few decades. However, the butanol is obviously suitable due to its properties: its higher energy content than ethanol induces a lower fuel consumption (up to 30%) and its lower water solubility decreases the tendency to microbial-induced corrosion in fuel storage and pipelines during transportation [11–13]. Moreover, the higher Cetane Number of butanol (CN = 25) compared to ethanol (CN = 8) leads to an easier auto-ignition in the case of CI engines [12]. It is also more suitable for diesel injection systems thanks to its higher level of viscosity, more like diesel fuel and no water content. Last, due to its very good miscibility with diesel without any co-solvents addition and the high oxygen concentration in the molecule itself, more and more studies about the butanol-diesel blends to improve Diesel engine performance and emissions can be found as reviewed Kumar et al. [2]. However, the brake specific fuel consumption increases with the proportion of butanol in the blend because of the lower heating value [15,16]. Therefore, to optimize pollutant emissions without significant penalty on engine performance, the engine control parameters, such as injection pressure and strategies, and dilution were investigated [16,17]. The combined effect of butanol addition (until 40% by volume) and high EGR level provides a longer ignition delay to reduce both local equivalence ratio and combustion temperature with as consequence drastic decrease of NOx emissions without drawback on soot, HC and CO emissions. The oxygen content in butanol molecule enhances the soot oxidation to limit the particle matter emission in comparison with regular diesel fuel [12,18]. Also, to achieve higher oxygen concentration in fuel, other kinds of the oxygenated biofuel blends, such as butanol-ethanol–diesel blend were investigated to evaluate combustion and pollutant emission impacts [14,17–19] with more benefit for PM-NOx trade off. By increasing butanol volume fraction (up to 40%) in diesel blend will induce longer ID and LOL, the higher resistance to auto-ignition will then lead to a better mixing rate before start of combustion and certainly an improvement in NOx and smoke emissions [19–21]. Last, butanol-diesel blends are considered also for advanced combustion modes of CI engines [1,22,23] due to its longer ignition delay, high oxygen content, and high volatility.

A fermentation intermediate from butanol production, the Acetone-Butanol-Ethanol (ABE) mixture, is recently estimated as a new potential alternative fuel for CI engines, due to similar physical and chemical properties to those of butanol [24,25]. By using Clostridium bacteria, Clostridium beijerinckii or Clostridium acetobutylicum, the fermentation of lignocellulosic hydrolysate sugars produces a mixture of ABE generally in a volume ratio of 3:6:1 [12,24,25]. ABE mixture needs to be distilled and dehydrated to extract pure butanol. Therefore, if ABE mixture can be used directly as fuel, the energy cost due to the separation would decrease. Change et al. [25] investigated the effect of the ABE-diesel blends on the engine performance and emissions. They found that ABE-diesel blends up to 30%v can reduce the soot precursors and PM. By adding water (0.5%v in ABE-diesel blends 20%v), the brake thermal efficiency can be enhanced up to 8.65% and PM, NOx, PAHs reduced up to 61.6%, 16.4%, and 31.1%, respectively. In another study [26], the ABE-water mixture was blended with biodiesel-diesel to control NOx and PM emissions. The results presented that the use of water containing-ABE-biodiesel-diesel blends could simultaneously reduce both PM and NOx up to 30.7% and 63.1%, respectively.

Wu et al. [12] investigated the effect of butanol-diesel and ABE-diesel blends on LL in a Constant Volume Preburnt. They found that the pure ABE (3:6:1) and butanol sprays are narrower and shorter than pure diesel one due to higher volatility values, especially at the lowest ambient temperature. In another study [27], various volume fractions of ABE(3:6:1) in diesel blends, (20, 50, and 80%v), were investigated on the spray and combustion characteristics. The results showed that LL decreases as a function of ABE proportion, but ABE20 and D100 have similar spray characteristics while ABE50 and ABE80 are shorter and narrower ones.

The combustion of two ABE mixtures (ratio between acetone, butanol, ethanol in ABE mixture of 3:6:1 and 6:3:1) blended with diesel was also compared with pure diesel [12,27,28]. They found that the liquid and flame lift-off lengths are shorter and longer than D100 respectively as a function of the ABE proportion. The longer ID and longer “gap” between liquid length and flame lift-off length of ABE mixture provide more time and space to favour droplets vaporization and mixing with ambient gas, also due to a better volatility. As the results, ABE-diesel blends not only promote soot oxidation due to the oxygen content but also lower soot formation itself.

Even if these studies present some results about the high potential of ABE and butanol diesel blends to reduce simultaneously soot and NOx, there is not yet a complete comparative study of these fuels on spray and combustion behaviours to understand better the effect of fuel properties. It is therefore the objective of this study. The single component surrogate, n-Dodecane (n-Do100) was chosen due to its similar characteristics than Diesel fuel. The ABE mixture used in this study is composed of 30%v of Acetone, 60%v of Butanol and 10%v of Ethanol, as the most usual mixture obtained from the intermediate fermentation of butanol production. Different blends of ABE mixture and the butanol with n-Do100 were selected: 20%v Acetone-Butanol-Ethanol (ABE20), 20%v Butanol (Bu20), 40%v Butanol (Bu40). Last, the fuels matrix, presented in Table 1 is completed by a blend of 20%v butanol and 20%v

Table 1
Fuel properties of alcohols in comparison with n-Dodecane [12,29–32].

Properties	n-Do100	Acetone	Butanol	Ethanol	ABE20	Bu20	Eth20	Bu40	Bu20Eth20
Molecular formula	$C_{12}H_{26}$	C_3H_6O	$C_4H_{10}O$	C_2H_6O	$C_{8.5}H_{18.6}O_{0.4}$[a]	$C_{8.9}H_{19.9}O_{0.4}$[a]	$C_{7.1}H_{16.1}O_{0.5}$[a]	$C_7H_{16}O_{0.6}$[a]	$C_{7.8}H_{18.3}O_{0.9}$[a]
Density at 15 °C (kg/m^3)	752.8	789	813.3	794.1	760.7	763.3	758.8	774.9	770.6
Viscosity at 15 °C (mm^2/s)	2.032	0.149	4.119	1.489	1.642	2.124	1.881	2.527	2.077
Lower heating value (MJ/kg) [12,29]	44.1	29.6	33.1	26.8	41.5[b]	41.8[b]	40.5[b]	39.5[b]	38.3[b]
Cetane number [30]	74	–	17	8	–	–	–	–	–
Boiling point (K) [31]	489	329	391	351	464[b]	468[b]	460[b]	448[b]	440[b]
Vapor pressure at 298 K (kPa) [31]	0.02	30.80	0.58	7.91	2.17[b]	0.14[b]	1.66[b]	0.25[b]	1.76[b]
Latent heat of vaporization at 298 K (kJ/kg) [31,32]	362	518	582	904	411[b]	409[b]	475[b]	454[b]	520[b]
Oxygen concentration (% by mass)	–	27.6%	21.6%	32%	5.2%	4.6%	7.3%	9.1%	11.7%
Stoichiometric mixture fraction, Z_{st} (–)	0.0460	–	–	–	0.0489	0.0485	0.0500	0.0512	0.0528

[a] Equivalent formula based on mole fraction.

[b] Properties estimated from mass fraction of single-component fuels in the alcohol blends.