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A comparative analysis on combustion and emissions of some next generation higher-alcohol/diesel blends in a direct-injection diesel engine

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ABSTRACT

Higher alcohols are attractive next generation biofuels that can be extracted from sugary, starchy and ligno-cellulosic biomass feedstocks using sustainable pathways. Their viability for use in diesel engines has greatly improved ever since extended bio-synthetic pathways have achieved substantial yields of these alcohols using engineered micro-organisms. This study sets out to compare and analyze the effects of some higher alcohol/diesel blends on combustion and emission characteristics of a direct-injection diesel engine. Four test fuels containing 30% *by vol.* of *iso*-butanol, *n*-pentanol, *n*-hexanol and *n*-octanol (designated as ISB30, PEN30, HEX30 and OCT30 respectively) in ultra-low sulfur diesel (ULSD) were used. Results indicated that ISB30 experienced longest ignition delay and produced highest peaks of pressure and heat release rates (HRR) compared to other higher-alcohol blends. The ignition delay, peak pressure and peak HRR are found to be in the order of (from highest to lowest): ISB30 > PEN30 > HEX30 > OCT30 > ULSD. The combustion duration (CD) for all test fuels is in the sequence (from shortest to longest): ISB30 < PEN30 < HEX30 < OCT30 < ULSD. Experimental mass fraction burned profiles fitted using the Wiebe's function revealed that the burning rate at the start of combustion is rapid for ISB30 followed by PEN30, HEX30, OCT30 and ULSD. From the emissions standpoint, NOx emissions decreased for all blends at low/medium loads but increased for PEN30 and HEX30 at high engine loads only. Smoke opacity is low for all blends due to their oxygenated nature and was of the order (from highest to lowest): ULSD > OCT30 > HEX30 > PEN30 > ISB30. HC emissions are high for ISB30 and PEN30 while it decreased favorably for HEX30 and OCT30. It was of the order (from highest to lowest): ISB30 > PEN30 > ULSD > HEX30 > OCT30. CO emissions of the blends followed the trend of smoke emissions and remained lower than ULSD with the following order (from highest to lowest): ULSD > OCT30 > HEX30 > PEN30 > ISB30.

1. Introduction

Diesel engines are more popular energy conversion devices because of their higher fuel conversion efficiency, higher torque capability, higher durability and lower hydrocarbon and carbon monoxide (HC & CO) emissions when compared to gasoline engines. Increasing concerns of fossil fuel depletion, oil-price volatility, burgeoning energy demands, global warming by GHG (green-house gases) emissions, toxic pollutants (smoke and NOx) and rigorous emission regulations are driving the scientific community to find alternative renewable biofuels for use in diesel engines. Recently higher alcohols have gathered interest among engine researchers to use them in diesel engines either as a neat fuel or as a blending component because they offer higher calorific value, higher cetane number, better blend stability and lower vapor pressure when compared to other widely-studied lower alcohols like ethanol and methanol. The term 'higher alcohol' refers to a series of straight and branched chain alcohols that consists of four or more carbon atoms like butanol (C_4), pentanol (C_5), hexanol (C_6), heptanol (C_7), octanol (C_8), dodecanol (C_{12}) and phytol (C_{20})

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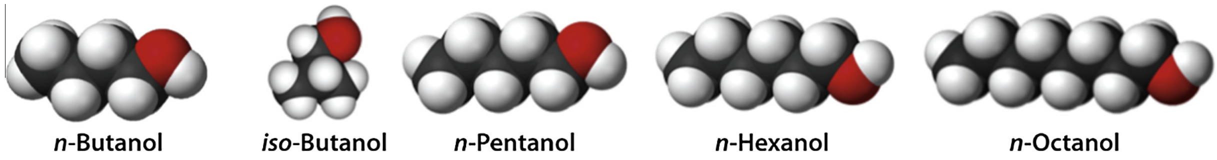

Fig. 1. Molecular structure of some higher alcohols.

Table 1
Properties of higher alcohols [1,5] in comparison with diesel and other lower alcohols.

Properties	Diesel	Methanol	Ethanol	*Iso*-Butanol	*n*-Pentanol	*n*-Hexanol	*n*-Octanol
Molecular weight (kg/kmol)	190–211.7	32.04	46.07	74.12	88.15	102.18	130.23
C (wt%)	86.13	37.48	52.14	64.82	68.13	70.52	73.72
H (wt%)	13.87	12.48	13.02	13.49	13.61	13.70	13.82
O (wt%)	0	49.93	34.73	21.59	18.15	15.70	12.29
Stoichiometric A/F ratio	14.67	6.47	9.01	11.21	11.76	12.15	12.71
Solubility (g/L)	Immiscible	Miscible	Miscible	77	22	7.9	4.6
Cetane number	52	5	8	<15	20	23	37
Self-ignition temperature (°C)	254–300	463	420	415	300	285	270
Density (kg/m^3) at 15 °C	835	791.3	789.4	802	814.8	821.8	827
Viscosity at 40 °C (mm/s^2)	2.72	0.58	1.13	2.63	2.89	4.64	5.8
Lower heating value (MJ/kg)	42.49	19.58	26.83	33.64	34.65	36.4	37.53
Latent heat of evaporation (kJ/kg)[a]	270–375	1162.64	918.42	684	647.1	603.0	545.0
Vapor pressure (mmHg)	0.4	127	55	10.4	6	0.928	0.08
Boiling point (°C)	180–360	64.7	78.3	108	137.9	157	195
Flash point (°C)	>55	11–12	17	28	49	63	81

[a] Data from Refs. [6,7].

Table 2
Microbial production of higher alcohols from engineered microbes with their yield.

Higher alcohol	Engineered host organisms	Source	Yield
Iso-butanol	*E. coli*	Glucose	22 g/L [9]
	E. coli	Glucose	50 g/L [12]
	Saccharomyces cerevisiae	Glucose	0.143 g/L [13]
	Clostridium cellulolyticum	Cellulose	0.66 g/L [14]
	Ralstonia eutropha	Formate	0.846 g/L [15]
	Corynebacterium glutamicum	Glucose	12.6 g/L [16]
	Synechococcus elongates	$CO_2 + H_2O$ + Light	0.45 g/L [17]
	Bascillus subtilis	Glucose	2.62 g/L [18]
n-pentanol	*E. coli*	Glucose	204.7 mg/L [11]
	E. coli	Glucose	2.22 g/L [19]
n-hexanol	*E. coli*	Glucose	302 mg/L [10]
	E. coli	Glucose	18.5 mg/L [11]
	E. coli	Glucose	47 mg/L [19]
	Clostridium carboxidivorans	Syngas	0.9 g/L [20]
	Clostridium acetobutylicum	Glucose	30 mg/L [21]
	Ralstonia eutropha	Glucose	280 mg/L [21]
n-octanol	*E. coli*	Glucose	62 mg/L [5]
	E. coli	Glucose	2 mg/L [10]
	E. coli	Glucose	70 mg/L [21]

[1]. The molecular structures of some higher alcohols are portrayed in Fig. 1.

Higher alcohols are found to be less corrosive on fuel injection and delivery systems due to their less hygroscopic nature than ethanol [2]. They have high flashpoints that offer safer storage and handling within the existing fuel distribution infrastructure. Their lower vapor pressures cause less evaporative emissions [3]. Though longer-chain alcohols have less oxygen content, they can still enhance the premixed combustion phase with their relatively longer ignition delays allowing sufficient mixing of air/fuel and also improve the diffusion combustion phase [1]. Furthermore, alcohols with longer carbon chains consume less energy during its production when compared to other lower alcohols since the biological process of breaking down large macromolecules can stop earlier [4]. The properties of higher alcohols in comparison with diesel and other lower alcohols are listed in Table 1.

The use of higher alcohols was earlier thwarted by high production costs, prolific use in food industry and limited production from non-petroleum resources [8]. Higher alcohols have never been able to be produced in larger quantities that make them potentially viable for use in diesel or gasoline engines until Atsumi et al. [9] achieved a high yield of 20 g/L of *iso*-butanol from glucose using the valine pathway in a lab-scale fermentor employing engineered *Escherichia coli*. Since then, bio-synthetic pathways have been extended to produce *n*-pentanol, *n*-hexanol, *n*-heptanol and *n*-octanol by employing larger substrates [10,11]. Table 2 provides the details of microbial production of these alcohols from engineered micro-organisms with their yield data.

It could be inferred from Table 2 that the last decade has witnessed a significant amount of research to produce greater yields of higher alcohols through biosynthesis. To complement these efforts, several experimental and chemical kinetic modeling studies have been carried out. Fundamental combustion studies on *iso*-butanol [22–27], *n*-pentanol [28–32], *n*-hexanol [30,33,34] and *n*-octanol [6,35] were conducted which included information on its oxidation, laminar burning velocities, flame structure,