LTC (low-temperature combustion) analysis of PCCI (premixed charge compression ignition) with n-butanol and cotton seed biodiesel versus combustion and emissions characteristics of their binary mixtures

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ABSTRACT

Direct injection (DI) of cotton seed biodiesel (CS100) with port fuel injection (PFI) of n-butanol was used for producing Premixed Controlled Compression Ignition (PCCI) to achieve low-temperature combustion (LTC) and obtain lower gaseous emissions in comparison to ULSD#2 (ultra-low sulfur diesel). PFI engine operation was compared to the combustion of binary mixtures of the same fuels reflecting the same weight ratio of high reactivity (CS100) and low reactivity (n-butanol) fuels. The supercharged engine was operated at constant speed and load with 20% exhaust gas recirculation (EGR). When compared to ULSD#2 reference, the ignition delay of 50% n-butanol and 50% CS100 binary mixture increased by 12% while the 50% n-butanol PFI with 50% CS100 DI led to a 17% decrease in ignition delay. Emissions of soot and nitrogen oxides were simultaneously improved using the PCCI strategy, reducing by 84% and 17%, respectively, given lower peak in-cylinder temperatures and increased oxygenation of the mixture. Carbon monoxide (CO) and unburned hydrocarbons (UHC) increased by several orders of magnitude as a downside of dual fuel injection; ringing intensity, however, improved, decreasing by 30% when using 50% n-butanol PFI in comparison to the ULSD#2 baseline given a smoother pressure gradients. Energy specific fuel consumption for CS50Bu50 (50% ULSD-50% n-butanol blend) increased by 4.5% compared to ULSD#2. The mechanical efficiencies and the coefficient of variation (COV) of IMEP were maintained at 70% and 2.5% respectively, during PCCI, indicating stable operation with renewable fuels.

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1. Introduction

Diesel engines are an essential part of modern transportation given their advantageous fuel efficiency. Engine operation, however, leads to emissions detrimental to the environment and human health. Strategies for control of in-cylinder diesel combustion have been proposed and pursued to allow proper control of such harmful emissions while minimizing costly implementation of aftertreatment systems. To reduce nitrogen oxides (NO_x) and particulate matter (PM) emissions, low-temperature combustion (LTC) modes have been developed through control of local mixture formation, ignition delay, and reactivity gradient at physical and chemical timescales. LTC modes such as Premixed Controlled Compression Ignition (PCCI) seek to obtain equivalence ratio

stratification across the cylinder, allowing for low temperature heat release as well as variable ignition delay. This will decrease the rate of pressure rise and allow for increased mixing time and duration of combustion [1].

Conventional high cetane diesel combustion would generally promote hydroxyl (•OH) production along with other radicals, which trigger a cool flame period before high temperature ignition during compression. Using a secondary fuel with lower cetane number such as a high carbon alcohol can be used to change the reaction pathways; the •OH formation can be decreased and consumption rates can be improved, leading to a beneficial combustion phasing and increased ignition delay. By retarding the cool-flame period, hot ignition and premixed combustion are delayed; the onset of high temperature oxidation is delayed in the effort of diminishing non-homogenous rich zones, which can cause an early ignition due to a higher concentration of hydrogen peroxide. This results in a decrease in maximum in-cylinder temperature

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subsequently reducing both PM and NO$_x$ [2]. Using two fuels of different reactivity will additionally allow for improved combustion control during PCCI operation [3]. The ratios of high to low reactivity fuels can then be varied to accommodate the combustion to a defined engine setup. Overall engine efficiency is additionally expected to improve given that an expanded combustion would result in more usable energy during the power stroke.

Various fuels have been considered for early port fuel injection (PFI) with direct injection (DI) of diesel. Gasoline PFI has been commonly investigated, namely with constant combustion phasing at sweeping injection timing. NO$_x$ was reduced by 30% and soot decreased by 90%, yet, carbon monoxide (CO) increased compared to conventional combustion, [4,5]. Double pulse direct injection of diesel would add more layers to the overall reactivity and utilize more available fuel energy for work and emissions reduction. E85 PFI has been compared to gasoline PFI at mid and high loads and has shown improvements in required EGR and indicated thermal efficiency. Lower PM and higher NO were achieved at a higher relative air-fuel ratio [6].

Alcohols, such as methanol and n-butanol, have also been implemented for PFI. n-Butanol PFI has shown simultaneous reduction in soot and NO$_x$ given better mixing and lengthened ignition delay. n-Butanol has been considered in this study over other alcohols, given its excellent miscibility with ULSD#2 (ultra-low sulfur diesel) and its higher energy content compared to other options, such as ethanol and methanol [7]. It has been shown to improve properties of biofuels in diesel combustion [8] as well as reducing smoke and NO$_x$ emissions when blended with diesel [9]. When increasing the n-butanol content in the mixture with biodiesel, it was shown to decrease overall carbon monoxide and unburned hydrocarbons while reducing NO$_x$ at high engine loads [10]. This further supports the production of n-butanol, which can be sustainable and more affordable than other biofuels. Butanol can be obtained from agricultural byproducts and waste [11,12], which would not directly affect main feedstock used for biofuel production.

In addition to emissions control, various other alternative fuels have been researched in the effort of supplementing the current petroleum diesel supply. LTC investigations have generally focused in paraffin fuel and small molecule kinetics. Renewable fuels such as biodiesel have been additionally investigated for their benefits in providing energy security as well as improving exhaust emissions. While studied as a replacement for ultra-low sulfur diesel (ULSD#2) in conventional diesel combustion and some LTC regimes for soot reduction [13,14], yet, biodiesel has to be comprehensively evaluated as a high reactivity fuel in place of conventional diesel in PCCI operation.

A study has investigated 20% soy FAME (fatty acid methyl esters) as the high reactivity fuel, which showed improvements in combustion efficiency at lower loads [15]. The resulting two stage heat release was controlled with less PFI fraction when compared to diesel. The combustion phasing allowed for reduction in particulate matter and NO$_x$. 100% peanut FAME was also operated with PFI of n-butanol, achieving LTC at low to medium loads [16]. Low temperature heat release along an overall lower peak heat release rate allowed for a maximum reduction of 98% in soot and 74% in nitrogen oxides.

This study sought to investigate FAME from cotton seeds as an alternative to ULSD#2 in PCCI. Cotton seed was selected to produce FAME given its high presence and availability to implement in the southern United States [17]. The abundance of cotton seeds for biodiesel would help meet EPA regulations for biofuel production and use [18]. Exhaust gas recirculation (EGR) was used given its ability to reduce various emissions simultaneously at low loads when coupled with low temperature combustion [19]. This is especially factual for NO$_x$ formation given decreased heat release rates [20] due to inert gases.

2. Thermo-physical properties of selected fuels

2.1. Fuel characteristics

Fuels' physical and chemical properties were evaluated given their significant influence on combustion and emissions characteristics. Properties of the selected fuels are shown in Table 1 n-Butanol was selected for its low cetane number and its high heat requirement for proper vaporization.

FAME from cotton seeds was produced in the lab using methanol with a sodium hydroxide catalyst. Quality per ASTM International standards was tested based on acidity as well residual methanol and glycerol content using an i-Spec biodiesel analyzer. The FAME profile of the Cotton Seed biodiesel was determined using a gas chromatography - flame ionization detector (GC-FID) to determine its molecular weight and cetane number. A linear regression model by Bambgoye and Hansen [22] and calibrated by Soloiu [16] was used based on the FAME composition of the transesterified cotton seed displayed in Table 2. Equation (1) was used for interpolation using variables x_2 to x_8 to symbolize fractions of the various FAMEs, the coefficients denoting lower cetane number with higher unsaturation. The calculated cetane number of 52 was similar to values reported in literature [23].

$$Cetane\ Number = 61.1 + 0.088x_2 + 0.133x_3 + 0.152x_4$$
$$- 0.101x_5 - 0.039x_6 - 0.243x_7 - 0.395x_8$$
(1)

The derived cetane number (CN) was determined for ULSD#2 and n-butanol using a PAC Cetane ID510 (available in the lab) following the ASTM method D7668-14a. The standard derived the cetane number by using the average ignition delay (ID) and combustion delay (CD) across 15 injection cycles in a constant volume, temperature controlled chamber which is detailed in Eq. (2). The CD is defined in this paper, as the period from start of injection (SOI) to the combustion pressure curve mid-point [24]. The chamber was operated at a mean pressure of 20 bar and wall temperature of 595 °C. The fuel was injected at 1000 bar for a duration of 2.5 ms.

$$CN = 13.028 - \frac{5.3378}{ID} + \frac{300.18}{CD} + \frac{3415.32}{CD^2}$$
(2)

Viscosity was investigated given its effect on spray atomization. Dynamic viscosity was determined from 20 °C to 60 °C using a Brookfield rotational viscometer (accuracy of ±1% FS) running with a spindle at 200 rpm. Cotton seed FAME (CS100) was found higher than ULSD#2 but was lower when blended with 50% n-butanol (CS50Bu50). The lower heating value (LHV) was also obtained, using a Parr constant-volume calorimeter. The LHV related to the energy released in-cylinder during combustion.

Table 1
Selected fuel properties.

Properties	ULSD#2	CS100	n-Butanol
LHV [MJ/kg]	42.6[a]	36[a]	33.1[a]
Cetane Number	47[a]	52[a]	15[a]
Density [g/cm^3]	0.84[a]	0.87[a]	0.80[a]
Dynamic Viscosity @ 40 C [cP]	2.4[a]	5.2[a]	1.8[a]
Molecular Weight [g/mol]	212[b]	292[a]	74[b]

[a] In authors' lab - experimental measurements,
[b] reference [21].