www.sphinxsai.com

ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN: 0974-4290
Vol.8, No.11 1 pp 292-299, 2015

Effects of Fuel Additive in HCCI combustion with Butanol Fuel Blends

S. Suthagar*, M.R.Swaminathan

Internal Combustion Division, Mechanical Engineering, College of Engineering, Guindy, Anna University, Chennai, Tamil Nadu 600025, India

Abstract: Homogeneous Charge Compression Ignition (HCCI) has attracted a great deal of interest as a combustion system for internal combustion engines because it achieves high efficiency and clean exhaust emissions. However, HCCI combustion has several issues that remain to be solved. This work investigates the benefits and challenges of enabling n-butanol and n-heptane in volume ratio of 80:20 with Hydrogen peroxide as ignition enhancer for HCCI combustion on a high compression ratio diesel engine. Minor engine modifications are made to implement port injection while other engine components are kept intact. The impacts of the fuel change, from diesel to n-butanol/n-heptane fuel blends with Hydrogen peroxide as additive is examined through steady-state engine tests. As demonstrated by the test results, the HCCI combustion of a thoroughly premixed fuel blend/air mixture offers ultralow NO_x emissions even without the use of exhaust gas recirculation and produces comparable engine efficiencies to those of conventional diesel high temperature combustion. The test results also manifest the control challenges of running an alcohol blend fuel in the HCCI combustion mode. The rapid heat release and the resultant excessive pressure rise rates prevent engine operation at higher loads, while a minimum level of intake boost is required to avoid misfire incidences at lower loads.

Introduction

Diesel engines have an excellent reputation for their low fuel consumption, reliability, and durability characteristics. They are also known for their extremely low hydrocarbon and carbon monoxide emissions. However, they have also been rejected by many for their odorous and sooty exhaust that is also characterized with high nitric oxide and particulate matter emissions. To capitalize on the merits on diesel combustion and to overcome the demerits, researchers are working on development of new combustion process called Homogenous charge compression-ignition (HCCI) combustion.[1] HCCI combines characteristics of conventional gasoline engine and diesel engines. Gasoline engines combine homogeneous charge with spark ignition (SI). Stratified charge compression ignition also relies on temperature and density increase resulting from compression. However, it injects fuel later, during the compression stroke. Combustion occurs at the boundary of the fuel and air, producing higher emissions, but allowing a leaner and higher compression burn, producing greater efficiency.[2]

The HCCI combustion clearly exhibits two-stage heat release, including a low-temperature heat release (LTHR, also referred to as low temperature reaction, cool-flame, or first-stage combustion) and a high-temperature heat release (HTHR, also known as high temperature reaction, hot flame, or second-stage combustion).Low-temperature reaction(LTR) has a significant influence on the High-temperature reaction (HTR).There are a number of obstacles that must be overcome before the potential benefits of HCCI combustion can be fully realized.[3] They are Homogenization mixture preparation, Combustion phase control, extending the operating range to high loads, Cold-start capability, Hydrocarbon and Carbon monoxide emissions. Although HCCI engines have been demonstrated to operate well at low-to-medium loads, difficulties have been encountered at high-loads. Combustion can become very rapid and intense, causing unacceptable noise, potential engine damage, and eventually unacceptable levels of NOx emissions.[4] HCCI ignition is determined by the charge mixture composition and its temperature history. Changing the power output of an HCCI engine requires a change in the fuelling rate and, hence, the charge mixture.

Fuel Additives and Blends In Hcci

PrimaryMain advantage of HCCI combustion is its intrinsic fuel flexibility. It is widely accepted that HCCI combustion is essentially dominated by the chemical kinetics of fuel/air mixtures under practical engine operating conditions. Fuel physical /chemical properties, as well as spatial and time histories, have dominant effects on ignition and combustion. Furthermore, a large number of studies have shown that traditional commercial fuels or sole-component fuels cannot meet the requirements for HCCI combustion.[5] Fuel additives, fuel blending, dual-fuel technology, and optimized fuel proportion in real-time can all be used to redesign the chemical kinetics.[6]

Butanol is a promising alcohol that combines the advantages of high energy density, high cetane number, strong hydrophobic properties and good atomization characteristics compared to other known oxygenate fuels like Ethanol. But n-butanol exhibits only single-stage ignition. No cool-flame or negative temperature coefficient (NTC) behavior has been observed from the oxidation of neat n-butanol.[7]When n-butanol is blended with n-heptane, it exhibited pronounced two stage ignition, indicating that the presence of n-heptane in the binary mixture promotes chain branching at low temperatures appreciably.[8] The stoichiometric ratio of the 80% n-butanol and 20% n-heptane is found to be 12.7 which is less when compared to the diesel fuel.[9]Hydrogen peroxide (H_2O_2) as additive would be expected to be a very effective accelerant because of its decomposition to form two reactive OH• radicals.[10] However, the bond dissociation energy of H_2O_2 is high (52 kcal/mole, 217 kJ/mole) corresponding to an activation temperature of 2615 K. This means that H_2O_2 doesn't decompose in the compression stroke until the temperature reaches around 900 K. Hydrogen peroxide decomposes into two OH radicals, which are very efficient at attacking the fuel and releasing energy.[11] The Stoichiometric Air fuel ratio of n-butanol (80%) and n-heptane (20%) by volume is found by following method.

$$0.8\,(nC_4H_9OH) + 0.2\,(nC_7H_{16}) + 7.4(O_2 + 3.76N_2) \rightarrow 4.6\,CO_2 + 5.6\,H_2O + 7.4\,(3.76\,N_2) \quad (1)$$

$$(A/F)_{Stoichio} = m_a/m_f \quad (2)$$

$$= 12.7$$

The heating value or calorific value of a combustible material is an important property, which may be used to evaluate its effectiveness for using as a fuel. . Heat of formation data is as follows for the above reaction

$\Delta H°_f$ of CO_2 (g)= –393.5 kJ/mol,
$\Delta H°_f$of H_2O(g) = –242.8 kJ/mol
$\Delta H°_f$ of n-C_4H_9OH (l)= –225.9 kJ/mol,
$\Delta H°_f$of n-C_7H_{16} (l) = –328.4 kJ/mol

$$\Delta H°_r = \sum_{Products} \Delta H°f - \sum_{Reactants} \Delta H°f \quad (3)$$

$$\Delta H°_r = -2910\ KJ/mol = -37\ MJ/kg$$

For the fuels covered in this study, n-butanol exhibits only single-stage ignition. No cool-flame or Negative Temperature Coefficient (NTC) behavior has been observed from the oxidation of neat n-butanol.[12]It is well-established that cool flame behavior is initiated through the dissociation of Ketohydroperoxides, which are produced via a sequence of low temperature oxidation steps in Equations 4 to 7.

$$R\cdot + O_2 \leftrightharpoons RO_2\cdot \quad (4)$$

$$RO_2\cdot \leftrightharpoons \cdot QOOH \quad (5)$$

$$\cdot QOOH + O_2 \leftrightharpoons \cdot O_2QOOH \quad (6)$$

$$\cdot O_2QOOH \leftrightharpoons \text{Ketohydroperoxides} + \cdot OH \quad (7)$$

Since n-butanol has a linear alkyl chain of four carbon atoms, one might expect that n-butanol would exhibit a certain extent of cool flame behavior based on the above-mentioned low temperature oxidation sequence.[13]

However, no noticeable cool flame behavior is observed in this study, suggesting that the presence of hydroxyl group in alcohols may help to promote certain chain-propagation channels that compete with the low temperature reactions in the chain-branching path. It is also found that the change of total ignition delay with compressed temperature does not follow a monotonic trend. Instead, Negative Temperature Coefficient behavior is observed for the B80 mixture.

Table I. Fuel properties

Property	Diesel	n-butanol	n-heptane
Chemical Formula	$C_{12}H_{26}$	n-C_4H_9OH	n-C_7H_{16}
Molecular weight	170	74	100
Latent heat of vaporization (kJ/kg)	270	430	316
Stoichiometric air/fuel ratio	14.7	11.1	15.4
Lower heating value of fuel	42.5	22.7	44.6
RON	-	92	-
MON	-	71	-
Density at 20° C (kg/m^3)	820-900	810	685
Auto ignition temp (°C)	210	385	223
Cetane Number	46-51	17	53

Experimental Seup

The experimental setup was equipped with instruments for observing performance, emission and combustion characteristics of the engine at different operating conditions. The schematic diagram and photographic view of the experimental setup are shown in Fig. 1. A single-cylinder, four-stroke, air-cooled, direct-injection, diesel engine with a displacement volume of 662 cm^3, developing 4.4 kW at 1500 rpm, was used for base line readings. The reason for selecting the diesel engine was that a high compression ratio can be easily employed for the HCCI mode. The engine always runs at its rated speed of 1500 rpm. The diesel engine was modified to work in the HCCI mode with port injector, fuel pump, fuel blending circuit and Electronic control unit.

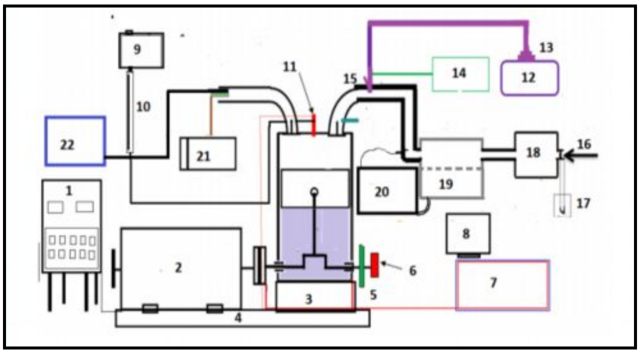
The Port Fuel Injector was mounted on galvanized intake port pipe. New intake port pipe was fabricated and also galvanized to prevent the corrosion due to alcohol injection. Injector and Port modification is explained in Fig. 2 .Since the usage of alcohols will cause hardware challenges to injector operation over the experiments. Extensive market study was carried out to find injectors capable of alcohol injections and BOSCH Gas Petrol Methanol injector was selected based on the flow capacity. The port fuel injector was controlled by an Electronic Control Unit (ECU). An electric pump has similar diaphragm-and-valve arrangement and a solenoid (an electromagnetic switch) provides the pull on the diaphragm. The solenoid attracts an iron rod that pulls the diaphragm down, drawing alcohol blend into the chamber.

Fuel pressure regulating circuit (Fig. 3) was fabricated with ideology to increase the pressure available at injector input as better atomization of alcohol blends will improve the combustion. The bench test was conducted with ECU by varying the injection pressure and injection duration to determine the fuel consumption. For each measured point, the pressure data of 137 cycles were recorded. The pressure data saved was fed to the Engine Combustion Pressure (ECP) analysis software to determine the Heat release rate, cumulative heat release rate, combustion mass rate, in-cylinder temperature, Indicated Mean Effective Pressure. Orifice plate with surge tank was used in this experiment to measure the air flow rate. A volumetric flow rate measurement was used when the conventional system was employed to inject diesel. The inlet air temperature and exhaust gas temperature was measured with the help of a K-type thermocouple capable of measuring temperatures up to 1200°C. Carbon monoxide (CO), Carbon dioxide (CO2), Nitrogen Oxide (NO) and Unburned Hydrocarbon (HC) were measured using AVL DIGAS 444 Non-Dispersive Infra-Red (NDIR) exhaust gas analyzer. The analyzer is based on the principle of selective absorption of the infrared energy of a particular wavelength peculiar to a certain gas, which will be absorbed by that gas. The instrument was periodically calibrated.

Experimenal Procedure

Experiments were performed at a constant speed of 1500 rpm at different load conditions. At each load, air flow rate, fuel flow rate, TDC position signals, cylinder pressure signals, HC, NO and CO emission readings were measured and recorded. Experiments were conducted to achieve the following.

1. Optimize the injection timing of the base diesel engine and obtain performance and emission characteristics in the standard diesel mode for comparison.
2. Study the effect of 80% n-butanol/20% n-heptane mixture by volume injection at the intake port on performance, emissions and combustion characteristics.
3. Study the effect of 80% n-butanol/20% n-heptane mixture with Hydrogen peroxide at the intake port on performance, emissions and combustion characteristics.
4. Optimize the injection characteristics of port injected alcohol blends for better performance, emissions and combustion characteristics in HCCI mode.
5. Optimize the HCCI engine emission parameters by trial and error.



1. Dyno controller	9. Fuel tank	17. Orifice meter
2. Dynamometer	10. Burette	18. Air box
3. Engine	11. Diesel Fuel Injector	19. Heater
4. Engine bed	12. Secondary fuel tank	20. Temperature controller
5. TDC sensor	13. Fuel pump	21. Exhaust gas analyzer
6. Encoder	14. ECU	22. Smoke meter
7. Data acquisition sys.	15. Port injector	
8. Computer	16. Intake air	

Fig. 1. Schematic diagram of Experimental setup

Fig. 2 Port injector setup

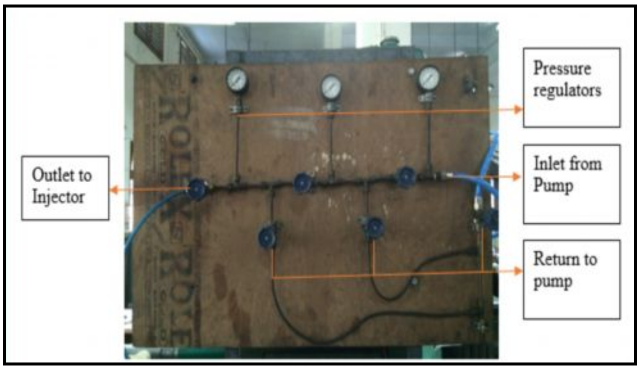


Fig. 3. Fuel pressurizing circuit

Result and Discussion

This part discusses the Performance of the engine when run using theAlcohol blend and N heptane mixture.

A. N-Butanol (80%)/N-Heptane (20%) (BH80) HCCI Combustion Characteristics.

Analysis of Cylinder pressure, heat release rate, in-cylinder temperature, Rate of pressure rise when engine is run with 80% n-butanol and 20% n-heptane (BH80) is discussed in the Fig. 4 to Fig. 7. When run in HCCI mode with BH80 fuel injected via intake port, we observe decrease in Cylinder pressure from neat diesel run a 0% Load. At 25% Load, BH80 undergoes uncontrolled combustion. Start of combustion advances with increase in load as per fundamentals, but controlled combustion behavior is not observed with standard operating conditions with BH80 fuel. High heat release rate shows intensity of rapid combustion for BH80 fuel. Also 2 Stage combustion behavior is not found with BH80 combustion from the heat release pattern. This supports the points that studied in the initial chemical kinetic study that rapid increase in gas temperatures will suppress the 2 stage ignition process. In-cylinder gas temperature follows the same trend of the Cylinder pressure is followed. From cylinder pressure traces at 50% load, increase in gas temperature corresponds to start of combustion. Average ROPR of BH80 fuel at various loads is compared and Maximum rate occurs for BH80 fuel in 50% load and this is above than 8 bar/deg which indicated ringing behavior. ROPR is less than 8 bar/deg at 25% load. At 0% load, ROPR is less than diesel curve indicating no combustion behavior.

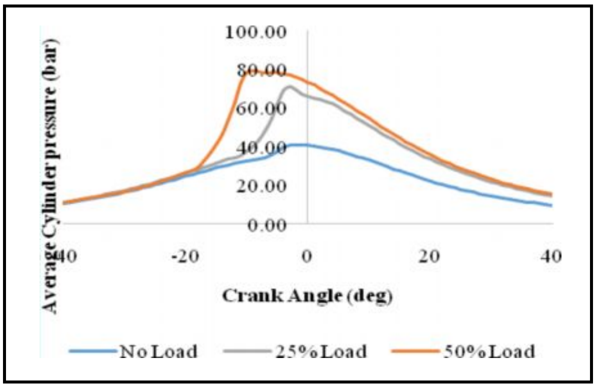


Fig. 4. Pressure crank angle comparison – BH80

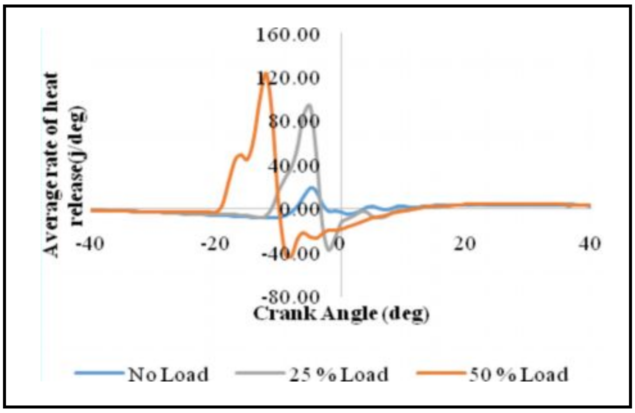


Fig. 5. Heat Release rate comparison – BH80

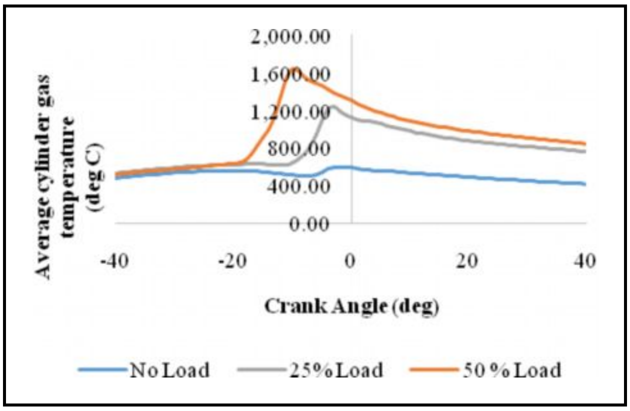


Fig. 6. Cylinder gas temperature comparison – BH80

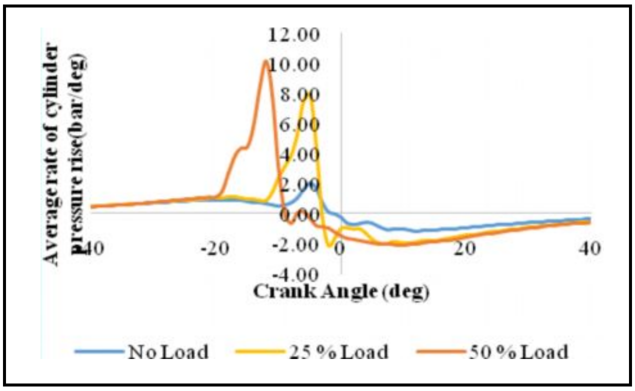


Fig. 7. Rate of Pressure Rise comparison – BH80

B. N-Butanol (80%)/N-Heptane (20%) with hydrogen peroxide (H_2O_2) HCCI combustion charateristics

Analysis of Cylinder pressure, heat release rate, in-cylinder temperature, Rate of pressure rise for BHM fuel blend is discussed in Fig. 8 to Fig. 11. At 0% load, maximum cylinder pressure occurs ATDC which is a favorable phenomenon. With BHM fuel, the combustion begins before top dead center which is desirable phenomenon. Peak pressure achieved increases with increase in load. This combustion phenomenon is very similar to HCCI combustion with 2 stage combustion. With H2O2 and chain propagation reaction initiated via n-heptane in BHM fuel mixture, combustion continues. Also presence of hydrogen peroxide advanced the start of combustion. Two stage combustion is observed in BHM mixture combustion. At 0% and 25 % load, LTC zone heat release rate is higher than the HTC zone. This is not desired as it will results in uncontrolled combustion. NTC zone presence is insignificant for these loads. At 50% load, perfect observation of 2 stage combustion is observed. It is observed that with BHM mixtures, In-cylinder temperatures drop below the diesel combustion temperatures after top dead center and this is due to 2 Stage combustion which occurs in HCCI combustion. Rate of pressure rise of BHM fuel blend is very similar to diesel mode pressure rise which indicates that the auto-ignition of the BHM mixtures in advance due ignition enhancers. Also combustion of mixtures due to Peroxide radicals' propagates in BHM. It is also observed that less than 8 bar/deg ROPR is observed with BHM fuels at all loads which indicates that, ringing behaviors exists but the intensity level is less.

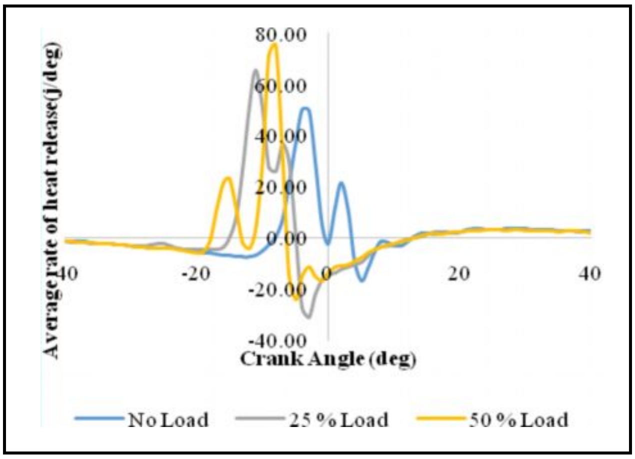


Fig. 8. Pressure crank angle comparison – BHM

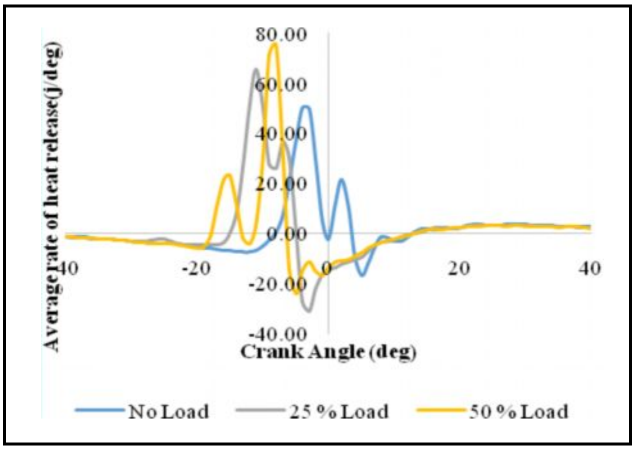


Fig. 9. Heat Release rate comparison – BHM

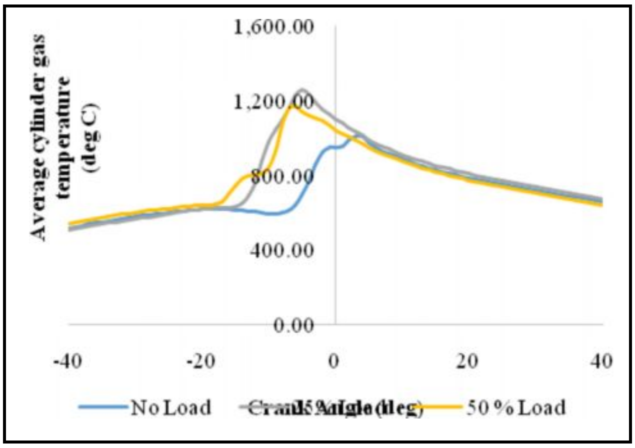


Fig. 10. Cylinder gas temperature comparison – BHM

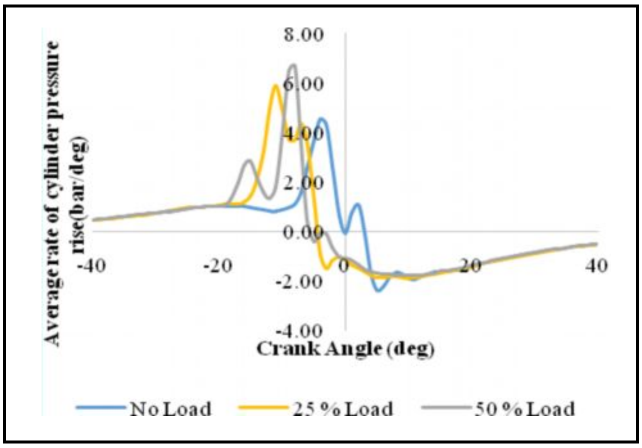


Fig. 11. Rate of Pressure Rise comparison – BHM

Brake thermal efficiency of HCCI runs is compared with neat diesel run at various load in Fig. 12. It is observed that the brake thermal efficiency of HCCI modes is less than the diesel run. This indicates that the fuel energy is not completely utilized. Also it can be observed that between the HCCI runs, BHM mixtures have higher brake thermal efficiencies when compared to BH80 fuel. This is evident from HCCI combustion characteristics comparison. Brake thermal efficiency of BHM fuel blend is 20% less than the diesel run at 25% load and 18% less at 50 % load. This is indicated with supporting conditions. Improving the combustion characteristics in HCCI mode will increase the brake thermal efficiency. Also Brake thermal efficiency increases in HCCI mode with decrease in equivalence ratio

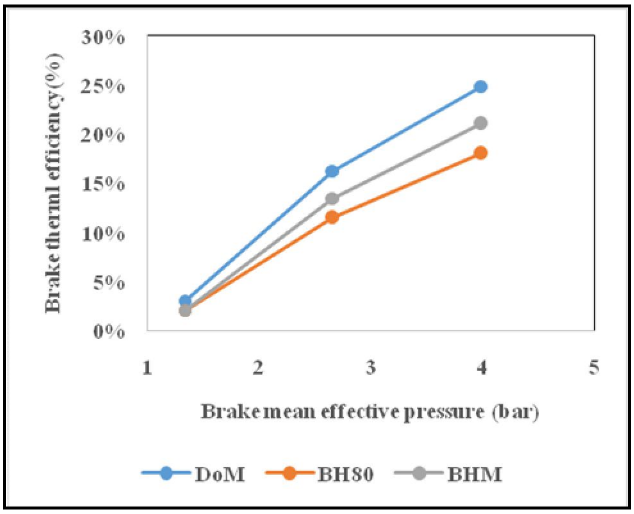


Fig. 12 HCCI Brake thermal efficiency

Conclusion

Experimental and theoretical investigation of homogeneous charge compression ignition combustion of diesel fuel with external mixture formation was carried out on a naturally aspirated, direct injection, single cylinder diesel engine. Two types Alcohol blend fuel mixtures namely BH80 and BHM were electronically injected at the intake port and the combustion, emission and performance characteristics of an adopted system were studied and presented. From the experiments conducted, the following conclusions were drawn.

- Initially, the test was conducted to study the performance, emission and combustion characteristics of the engine running with diesel fuel. Performance parameters were studied and from the study, it was found that engine is capable of running at ~ 28 % brake thermal efficiency at full load which compared with the historical data.
- HCCI Combustion parameters were studied and from the study, it was found that engine is capable of running between 0% Load and 50% Load with standard operating conditions. Also 0% load operations was difficult and the same holds true for oad above 50%. The reason being Misfire at 0% load and knocking for more than 50% load.
- For BH80 fuel, 2 stage combustion was not observed at all loads.
- The heat release rate at 50% load for BHM fuel clearly indicates the occurrence of Low temperature reactions (LTR) followed by a zone of High temperature reactions (HTR). The start of combustion was influenced by the start of low temperature reactions. Also due to presence of Hydrogen peroxide, reactivity of the BHM mixture increases.
- Brake thermal efficiency decreases with BH80 and BHM fuel blends. Brake thermal efficiency decreases by 20% at 50% load and by 25 % at 25% load. This indicates that efficiency can be increases with improvised operating conditions.

References

1. C. Weiskirch , M.Kaack , L.Blei and P.Eilts “Alternative Fuels for Alternative and conventional Diesel Combustion systems” SAE 2008-01-2507.
2. Thomas W . Ryan III and Andrew C. Matheaus "Fuel Requirements for HCCI Engine Operation" , SAE 2003-01-1813.
3. Gen Shibat,Tomonori Urushihara "Auto-Ignition Characteristics of Hydrocarbons and Development of HCCI Fuel Index " SAE 2007-01-0220.

4. LÜ Xingcai, JI Libin, ZU linlin and HUANG Zhen "Numerical simulation and experimental study on the n-heptane HCCI combustion with port injection of reaction additive ", SAE-2007-01-1875.
5. Scott D. Schwab, Gregory H. Guinther, Timothy J. Henly and Keith T. Miller. "The Effects of 2-Ethylhexyl Nitrate and Di-Tertiary-Butyl Peroxide on the Exhaust Emissions from a Heavy-Duty Diesel Engine" SAE 1999-01-1478.
6. Hiroaki Nomura, Takuya Muto, Sayaka Nishimi and Kazunori Yoshida " Influences of Compression Ratio and Methane Additive on Combustion Characteristics in a DME-HCCI Engine " SAE-2005-01-3745.
7. J. Hunter Mack , Robert W. Dibble , Bruce A. Buchholz and Daniel L. Flowers "The Effect of the Di-Tertiary Butyl Peroxide (DTBP) additive on HCCI Combustion of Fuel Blends of Ethanol and Diethyl Ether " SAE-2005-01-2135.
8. G. Gnanam, A. Sobiesiak and G. Reader and C. Zhang " An HCCI Engine Fuelled with Iso-octane and Ethanol" , SAE-2006-01-3246.
9. P. Saisirirat1, F. Foucher,S. Chanchaona and C.Mounaïm-Roussell "Effects of Ethanol, n-Butanol – n-Heptane Blended on Low Temperature Heat Release and HRR Phasing in Diesel-HCCI" SAE 2009-24-0094.
10. Salvador M.Aceves , Daniel flowers , Joel Martinez-Frias, Franscisco Espinosa-Loza , William J.Pitz "Fuel and Additive Characterization for HCCI combustion" , SAE 2003-01-1814.
11. Shigeyuki Tanaka , Ferran Ayala , James C.Keck , John B Heywood "Two-Stage Ignition in HCCI combustion and HCCI control by fuels and additives " Combustion and Flame 132 (2003) 219 – 239
12. Ashutosh Gupta, David L. Miller and Nicholas P. Cernansky" A Detailed Kinetic Study on the Effect of DTBP on PRF Combustion in HCCI Engines " SAE 2007-01-2002.
13. Xiaohui Gong, Rodney Johnson, David L. Miller and Nicholas P. Cernansky "Effects of DTBP on the HCCI Combustion Characteristics of SI Primary Reference Fuels " SAE - 2005-01-3740.

*****