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Performance and Emission Characteristics of Heptane/Toluene Blends at Constant Injection Operation on a CI Engine

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Abstract

Hydrocarbons are chemical compounds whose molecules are made of hydrogen and carbon. Heptane is an aliphatic hydrocarbon with good ignition quality and high cetane number, while Toluene is an aromatic hydrocarbon with a very poor ignition quality and very low cetane number. The two different compounds are blended in varying proportion and tested in a single cylinder 2.0L Ford Puma automotive diesel engine to investigate their effect on engine performance and emission. The cylinder pressure, heat release rate, exhaust gas emissions and particulate were measured. The results show that H70T30 blend has the highest specific NO_x emission which was due to the high peak temperature and produces slightly more soot than pure heptane (H100T0). H50T50 attained the lowest heat release rate, peak cylinder pressure and temperature. These low values favour the formation of low NO_x, high amount of unburned hydrocarbon and high amount of soot particles. Although heptane has a high cetane number, it fails to act as an ignition improver to toluene.

Keywords: Hydrocarbon, Heptane, Toluene, Blend, Constant Injection, CI Engine

1. Introduction

Hydrocarbons are organic chemical compounds that contain only carbon (C) and hydrogen (H). The hydrocarbon molecule is built upon a skeleton of carbon atoms bonded to each other either in the form of closed rings or in a continuous row-like links in a chain. The carbon atoms chain may be either straight or branched. In all cases, whether it is ring or chain, straight or branched, all the hydrogen atoms are attached to the carbon bonds that have not been used in tying carbon atoms together in the carbon skeleton. The fact that there is apparently no limit to the size and complexity of the carbon skeletons, there is therefore no limit to the number of different hydrocarbons that can exist [1]. Hydrocarbons, on the basis of their sources and properties are classified as either aliphatic or aromatic. Aliphatic is the hydrocarbons derived from the chemical degradation of fats or oils. They are either saturated or unsaturated. The aromatic hydrocarbons are a group of related substances obtained by chemical degradation of certain pleasant-smelling plant extracts [2-5]. They are either alkylated or non-Alkylated. According to Murphy and McCormick (2004), cetane number (CN) of a blend of fuels is a linear combination of the cetane numbers of the components. $[BlendCN = \text{molar fraction of fuel A}(\text{CN of fuel A}) + \text{Molar fraction of fuel B}(\text{CN of fuel B})]$ [6]. Kwon et al in 2003 determined experimentally the diffusion coefficient for some hydrocarbons and observed that toluene at 24.6^oC and 1atm with heptane at 24^oC and 1atm have diffusion coefficient of 0.0859cm²/s and 0.0734cm²/s respectively. These values imply that under the same condition toluene has a greater tendency of diffusing faster by 0.0125cm²/s out of the mixture relatively to heptane [7]. Ciniviz *et al* 2011 carried out an experimental investigation of the effect of methanol blended diesel fuels on engine performance and observed that the brake specific fuel consumption and nitrogen oxide emissions increased while brake thermal efficiency, carbon monoxide and hydrocarbons decreased relative to single diesel fuel operation with increasing amount of methanol in the fuel mixture [8]. Many other researchers reported on the benefit of blending ethanol with diesel fuel [9-19]. In their investigation on the performance and emission characteristics of diesel engine fuelled with ethanol-diesel blend, Lei *et al* (2011) determined experimentally that the equivalent brake-specific fuel consumption (BSFC) of ethanol-diesel blends are better than that of diesel under different atmospheric pressures and that the equivalent BSFC gets great improvement with the rise of atmospheric pressure when the

atmospheric pressure is lower than 90 kPa [20]. The investigations on blended hydrocarbons show a positive improvement in engine performance. It is worth noting that most of the experiments conducted were on hydrocarbons with good ignition qualities.

In this paper, heptane (aliphatic hydrocarbons) is blended with toluene (aromatic hydrocarbons) to examine the influence of a better ignition quality fuel (heptane) on a poor ignition quality hydrocarbon (toluene). The basis for the analysis was strictly the percentage concentration of heptane in toluene and its resultant effect as fuel on engine performance and emissions. Heptane is a straight chain aliphatic hydrocarbon of seven carbon atoms and sixteen hydrogen atoms having a molecular formula of C_7H_{16} . It is colourless liquid which is soluble in water. Toluene is an aromatic hydrocarbon with one benzene ring and a methyl group. It consists of seven carbon atoms and eight hydrogen atoms. It is clear water- soluble liquid with a typical smell of paint thinner which is quite dangerous for human inhalation and could cause neurological harm.

2. Materials and Methods

2.1 Experimental Apparatus

A single cylinder direct injection common rail research engine with an electronically controlled solenoid injector based on Ricardo Hydra engine was used for the experiment. The engine was a 2.0L Ford Puma™ with an automotive compression ignition engine and a compression ratio of 15:1. The external exhaust has a gas recirculation system with optional cooling in the homogenous charge compression ignition (HCCI). A naturally aspirated air flow was used for the engine. The crank angle was monitored with an optical shaft encoder driven directly by the engine crankshaft at 1800 pulses per revolution. A Kistler™ 6056AU38 piezoelectric pressure transducer and a Kistler™ Type 5011 charge amplifier was used to record the cylinder pressure at a constant interval of 0.2 degree crank angle. The exhaust gas emissions were measured using four different sensors/detectors. The chemi-luminescence detection (CLD) was used to measure the NO_x emission, the non-dispersive infrared sensor (NDIR) for CO and CO₂ emission, the flame ionization detector (FID) for the unburned hydrocarbon emission and magneto-pneumatic detection (MPD) for the O₂ emissions at the exhaust. The Cambustion DMS500™ fast particulate spectrometer can measure particles of the order of 5-2500nm was used to measure the quantity and size of the particulates. The test rig for the experiment is shown in figure 1.

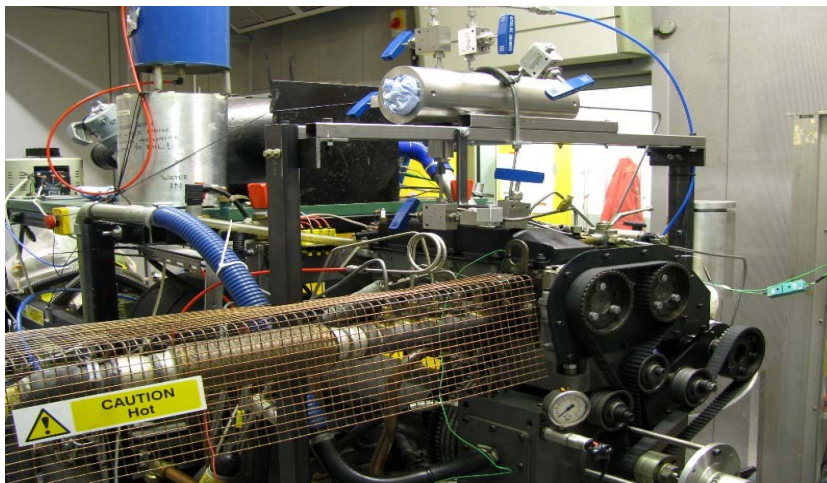


Figure 1. The test rig (The 2.0L Ford Puma Engine)

2.2 Experimental Procedure

The experiment was conducted at 1200 rpm, with a corresponding to 0.4 MPa IMEP output and an injection pressure of 45 MPa. At the beginning of the experiment, the piston in contact with fuel sample was removed by blowing in a highly pressurized fuel from the compressed air line in the laboratory through one of the port located on the cylinder. In order to avoid contamination, the piston was removed and cleaned. The test samples was fed in through the funnel into the left chamber of the cylinder and bled to displace any amount of air trapped in the cylinder. Also the valve leading from the ultra-low volume cylinder into the injector was opened and all other valves were shut. The fuel system was held at a constant temperature of $353\text{ K} \pm 2\text{ K}$. The heating system was controlled by an electronically proportional-integral-derivative (PID) installed on the fuel injection system. The engine dynamometer control system was used to motored the engine to the required speed after the pressure connections and valves were secured. The injection timing for the small fuel test sample and the pressure of the common-rail were adjusted electronically via the engine control system [21,22].

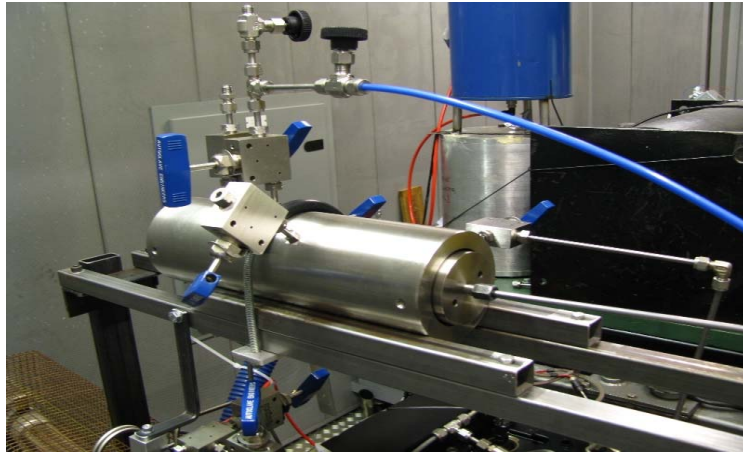


Figure 2. Ultra low volume fuel system

2.3 The Test Fuels Properties

The test fuel was a mixture of a straight chain aliphatic (heptane) and aromatic (toluene) hydrocarbon in varying proportion. The varying proportion of toluene and heptane was decided in molar ratios while the preparation and mixing of the two hydrocarbons was done gravimetrically. The gravimetric analysis made it possible to determine the mass equivalent of the molar proportion and mix accordingly as shown in table 2. Figure 3 shows the molecular structures of heptane and toluene while table 1 shows the details of the properties of the two hydrocarbons.

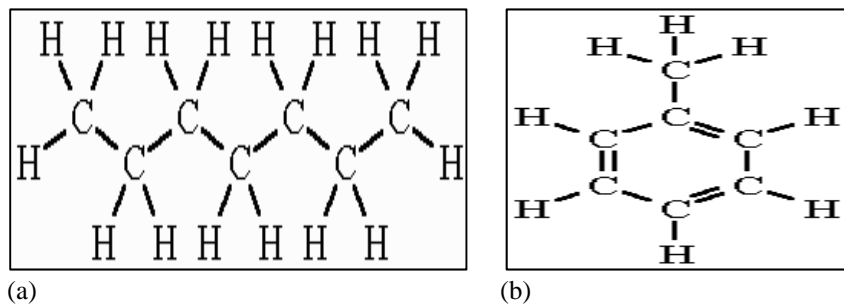


Figure 3. Molecular structure of Heptane (a) and Toluene (b) [23,24]

Table 1. Properties of Test Fuel

Properties	Heptane	Toluene
Lower heating value (KJ/Kg)	44.566	40.589
Density (g/mL)	0.684	0.865
Cetane number	52.5,53,56	-5,9,18.3
Normal boiling point (°C)	98	110-111
Melting point (°C)	-91	-93
Carbon composition by weight (%)	83.89	91.24
Hydrogen composition by weight (%)	16.12	8.76
Molecular weight (g/mol)	100.20	92.14
Flash point (°C)	-4	4
Autoignition temperature (°C)	215	536
Purity level (%)	99	99.8

Table 2. Mixture samples data

Molar proportion		Mass (grams/100mL)		Volume (mL)	
Heptane	Toluene	Heptane	Toluene	Heptane	Toluene
100	0	68.400	0	100	0
70	30	52.150	20.550	76.243	23.757
50	50	39.605	36.415	57.901	42.099
45	55	36.216	40.700	52.948	47.052

2.4 Experimental Condition

The test was conducted under constant injection timing where the base diesel was used as the reference. The ignition delay which is strongly dependent on the molecular structure of the fuel was also equalized by addition of 2-ethylhexylnitrate for base diesel, H70T30 and H40T60 to eliminate the effect of ignition delay on the combustion process. This answers the question of how the mixtures will behave should the physical fuel and air mixing be similar. Table 3 gives a summary of the test conditions.

Table 3. Constant injection timing

Test fuel	IMEP MPa	Engine speed (RPM)	Injection timing (BTDC)	Ignition timing (BTDC)	Injection pressure (MPa)	Injection time (μ s)
Diesel en590	0.4	1200	6.5	TDC	45	810
H100T0	0.4	1200	6.5	0.4	45	794
H70T30	0.4	1200	6.5	-0.8	45	712
H50T50	0.4	1200	6.5	-2.8	45	847
H45T55	0.4	1200	*	*	45	
Diesel en590	0.4	1200	6.5	TDC	45	765

Where * means "did not combust"

3. Experimental Results

In other to ensure that the properties of the combustion chamber was held constant at point of injection. All test fuels were injected at the same timing as that of the base diesel. Figure 4 shows the cylinder pressure, figure 5 shows the heat release rate, figure 6 shows the mass fraction burnt, figure 7 shows the specific emissions and figure 8 shows the size spectral density.

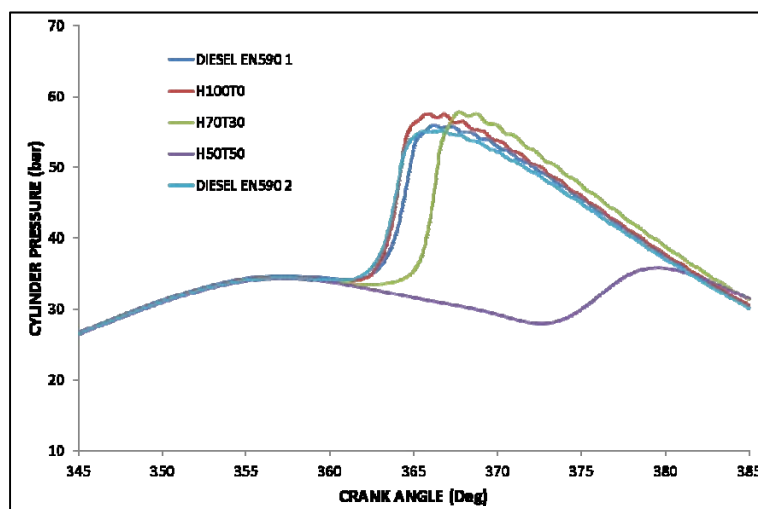


Figure 4. Cylinder pressure against crank angle at constant injection timing

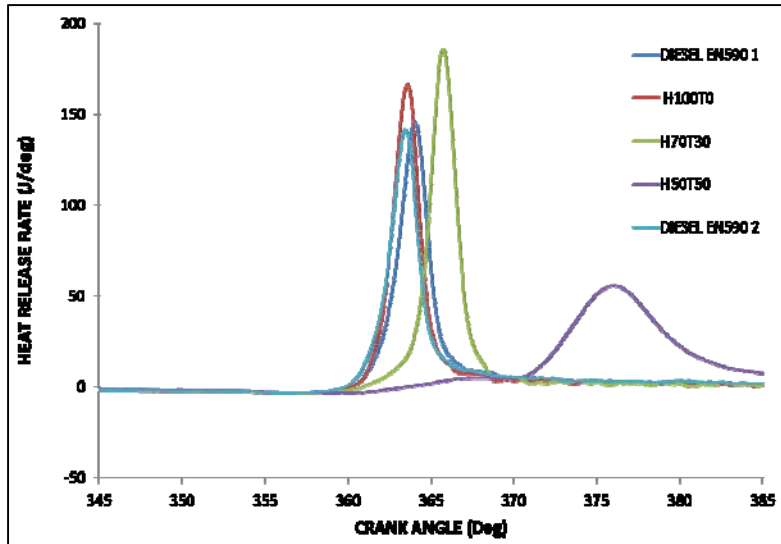


Figure 5. Heat release rate against crank angle at constant injection timing.

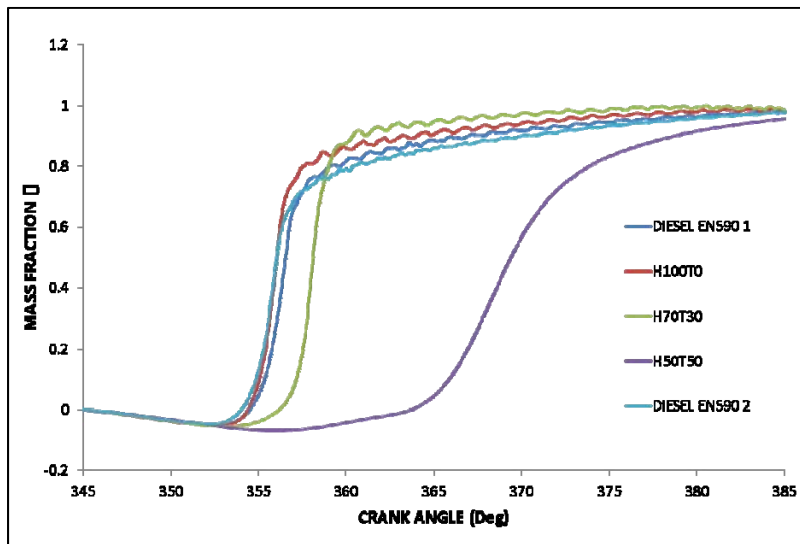


Figure 6. Mass fraction against crank angle at constant injection timing

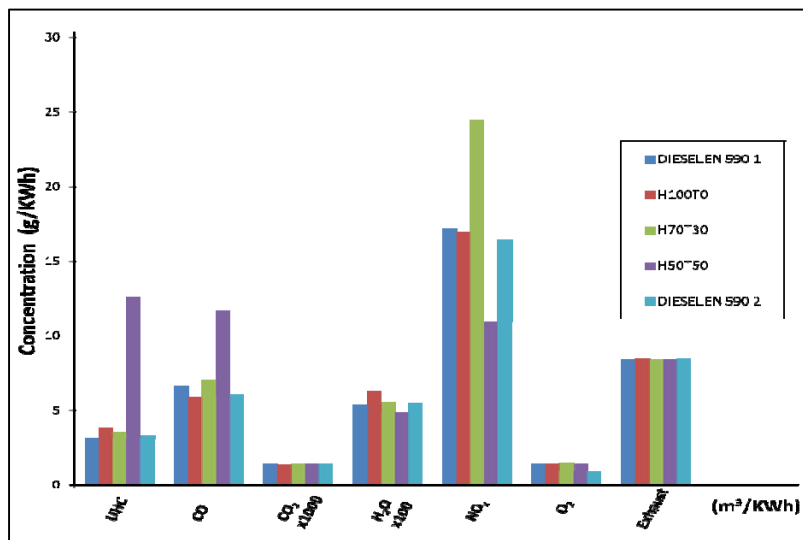


Figure7. Specific emissions at constant injection timing

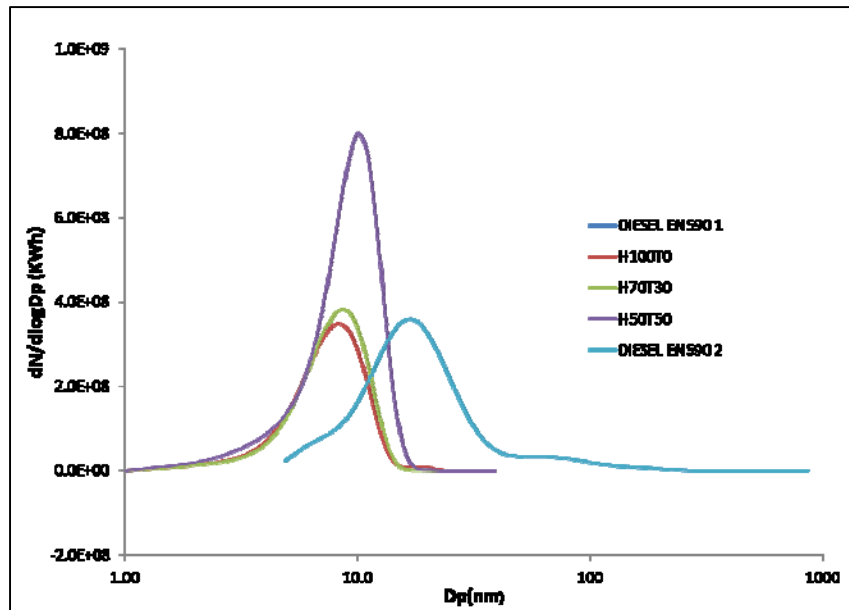


Figure 8. Size spectral density at constant injection timing

4. Discussions

The H70T30 has almost the same peak cylinder pressure as H100T0 but due to better ignition quality of H100T0, the ignition of H100T0 began much earlier than that of H70T30 (figure 4). There was little or no effect of heptane on toluene in terms of cylinder pressure at H70T30. With H50T50 there is no influence of heptane on toluene as the fuel refused to combust. The peak heat release rate for H70T30 was however higher than H100T0 which is justified because of the higher ignition delay and hence a more premixed phase combustion than pure heptane (H100T0) which had more of diffusion controlled combustion (figure 5). H70T30 also has the highest specific NO_x emission which was due to the high peak temperature which always favours the formation of NO_x . It produces slightly more soot than pure heptane (H100T0). H50T50 attained the lowest heat release rate, peak cylinder pressure and temperature (figure 6 and figure 7). These low values favour the formation of low NO_x , high amount of unburned hydrocarbon and high amount of soot particles. The exceptional high amount of particulates (figure 8) and soot is a combined effect of reluctance to combustion and high dominance effect of toluene in the mixture. This is against earlier concept that heptane being of higher ignition quality will acts as cetane improver. The unburned hydrocarbon upon coalescence adheres to the soot to form an increase amount of particulate matter. The fact that during the experiment H40 T60, H45T55 and H35 T65 failed to combust at constant injection timing shows that the high ignition quality of heptane has little or no influence on toluene which has very poor ignition quality. It has been earlier presupposed that a compound of good ignition quality acts as an ignition improver in a binary mixture for a compound of poor ignition quality. This however has not been the case as the above has shown. The reason for the lack of effect of heptane on toluene is justified from the experiment conducted by Kwon et al in 2003 as stated in the literature that under the same condition, toluene has a greater tendency of diffusing faster by $0.0125\text{cm}^2/\text{s}$ out of the mixture relatively to heptane. Toluene diffuses out of the atomized droplet of fuel mixture and accumulates at the boundary phase of the droplets with air. The boundary rich in toluene acts a point of first contact with the air in the cylinder.

5. Conclusion

A good ignition quality hydrocarbon (Heptane) was successful blended with a very low ignition quality hydrocarbon (Toluene) at different proportions. The blends were tested in a single cylinder 2.0L Ford Puma automotive diesel engine operating at constant injection, to investigate their effect on engine performance and emission. The cylinder pressure, heat release rate, exhaust gas emissions and particulate were measured. The results show that H70T30 blend has the highest specific NO_x emission which was due to the high peak temperature and produces slightly more soot than pure heptane (H100T0). H50T50 attained the lowest heat release rate, peak cylinder pressure and temperature. These low values favour the formation of low NO_x , high amount of unburned hydrocarbon and high amount of soot particles. It was also observed that the toluene exercised a higher degree of dominance on the heptane. This is evident on the sharp difference that existed between H100T0 and H70T30. On the other hand the mixture H60T40 and H70T30 did not combust in spite of the considerable presence of heptane.

Acknowledgement

The authors will like to thank the Petroleum Technology Development Fund (PTDF) for providing the research fund on behalf of the Federal Government of Nigeria. The invaluable suggestions and contributions from Prof N. Ladommatos of University College London during the research work were highly appreciated.

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