Modeling and Analysis of the Relationship of Octane, Cetane and Ignition Delay Usage

Kamalu C.I.O
Department of Chemical Engineering, Federal University of Technology, Owerri, Nigeria.

Iwot O.A
Department of Chemical Engineering, Federal University of Technology, Owerri, Nigeria.

Okere P.C
NNPC/PPMC, Port Harcourt Depot, Alesa Eleme, Rivers State, Nigeria.

Ogah A.O
Department of Food Science and Technology, Federal University Ndufu-Alike, Ikwo, Ebonyi State, Nigeria.

Obijiaku J.C
Department of Chemical Engineering, Federal University of Technology, Owerri, Nigeria.

Abstract – This work successfully modeled and validated the relationship between octane number and cetane number for conversion from diesel to petrol engine and vice versa. The Ignition Quality Tester (IQT) was used to carry out combustion experimental work on diesel fuel involving Ignition delay - temperature relationship as well as ignition delay - pressure relationship. The same was used to determine cetane number - ignition delay, %volume additive - increase in cetane number and octane number - cetane number relationships. Tests were conducted at constant pressure and temperatures of 145psi and 828K respectively. Experimental data were curve-fitted at R^2 of 0.9982%, 0.9952%, 0.9954%, 0.9937% and 0.9991% for ignition delay - pressure, %volume 2-EHN additive - increase in cetane number, cetane number - ignition delay, ignition delay - temperature, and octane number -cetane number experiments respectively. The experimental data agree very well with derived models and in real life. Model validation accuracy for the combustion relating to octane-cetane relationship gives R^2 value of 0.9991 which affirms that experimental data agree well with the derived model. The work can be utilized in automobile industry to ascertain the equivalence of converting from one fuel to the other vis-à-vis octane and cetanes based fuels and also correlate variable parameters in fuel combustion as the case may be.

Index Terms – Modeling, octane, cetane, ignition delay, relationship.

1. INTRODUCTION

Simply put, the octane rating of the fuel reflects the ability of unburned end gases to resist spontaneous auto-ignition under the engine test condition used.

If auto-ignition occurs, it results in an extremely rapid pressure rise, as both the desired spark-initiated flame front and the undesired auto-ignited end gas flame expand. The combined pressure pick arrives slightly ahead of the normal operating pressure peak leading to a loss of power and saw tooth pattern of pressure oscillations that create the "knocking" sound. The combination of intense pressure waves and overheating can induce piston failure in a few minutes. Knock and pre-ignition are both favoured by high temperature, so that one may lead to the other. Under high speed conditions, knock can lead to pre-ignition which then accelerates engine destruction (Taylor, 1994).

The octane rating of hydrocarbon is determined by the structure of the molecules, with long straight hydrocarbon chains producing large amounts of easily auto-ignitable pre-flame decomposition species, while branched and aromatic hydrocarbons are more resistant. This also, explains why the octane ratings of paraffins consistently decrease with carbon number (Taylor and Michael, 2004).

The addition of an additive such as alkyl lead and oxygenates can significantly affect the pre-flame reaction pathways. Anti-knock additive work interfering at different points in the pre-flame reaction, with the oxygenates restarting undesirable low temperature reactions, and the alkyl lead compound react in the intermediate temperature region to deactivate the major undesirable chain branching sequence. The anti-knock ability is related to the "auto-ignition temperature" of the hydrocarbon (Ryan and Calahan, 2009).

The octane number of a fuel is based on how fuel auto-ignite, under compression. It is based on the scale where isooctane is given the number given the number 100 (minimal under pressure) while hexane is given the number zero (easily ignite under pressure). For example, a petrol with octane number of

92 has the same knock as a mixture of 92% isooctane and 8% hexane. Octane rating decreases with increase in carbon chain length while it increases in aromatics with same numbers of carbon. It is important to know the octane number for petrol because the auto-ignition of fuel causes a knocking effect. In petrol engine, it ignites twice “once due to high pressure and again when the spark ignite the petrol”. This causes the car engine to be less efficient and can also damage the engine (Phoung et al., 2000). However, diesel engines rely on knocking-effect as they have no spark plugs and rely on the effect of compression to make the fuel and air mixtures ignite. There are two (2) ways to increase the octane number of a fuel. “One is to put special additive into the fuel which discourage auto-ignition and the other is to blend high octane fuel i.e with ordinary petrol. Anti-knocking additive are substances which reduce the tendency of a fuel to auto-ignite and so increase the octane number (Challen and Barneseu, 1999).

Cetane number is the measurement of combustion quality of diesel fuel during compression ignition. Thus, it is the approximate equivalent of octane rating in gasoline (petrol). The cetane number is an important factor in determining the quality of diesel fuel but not the only one (Boerlage and Broeze, 1932).

Other measurements of diesel quality includes; density, lubricity, cold-flow, properties and sulphur content. “Cetane number is a measure of a fuel ignition delay, the time period between the start of ignition and the first identifiable pressure increase during combustion of fuel. In a particular diesel engine, high cetane fuel will have shorter ignition delay period than lower cetane fuel. In short, the higher the cetane number, the more easily the fuel will combust in the compression cetane (such as a diesel engine). The characteristics diesel “knock” occurs when the first portion of the fuel that has been injected into the cylinder suddenly ignites after an initial, minimizing this delay result in less unburned fuel in the cylinder at the beginning as less instance knock (Brewster and kerly, 1963).

Therefore, high cetane fuels usually cause the engine to run more smoothly and quickly. This does not necessarily translate into greater efficiency, although it may in certain engine.

Generally, diesel engines operate well with a cetane number of 40 to 55. Fuel with higher cetane number has shorter ignition delay not enough for the fuel combustion process to be completed.

The higher speed diesel engine operates more efficiently with the higher cetane number fuel. Alkyl nitrate (principally 2-ethylhexyl nitrate) and di-tri-butyl peroxide are used as additive to cetane number (Baxleg and Rendel, 1931).

Cetane is a chemical compound; alkane (named hexadecane IUPAC rules chemical formula n-$C_{16}H_{34}$) molecules of which are unbranched and with open chain. Cetane ignite very easily under compression. It was assigned a cetane number of 100 while alpha-methyl naphthalene was assigned a number of zero (0). All other hydrocarbons in diesel fuel are indexed to cetane as to how well they ignite under compression. The cetane number, therefore, measures how quickly the fuel starts to burn (auto-ignites) under diesel engine conditions (Urban and Gray, 1968).

The relationship between cetane and octane number for diesel vehicle that are to be converted to gasoline vehicle has been discussed extensively in the literature and how it will relate to ignition delay is the essence of our discussion.

Vehicles these days are converted from one form of fuel to another, traversing between cetane and octane number application and of certain ignition delay phenomena.

The octane number of gasoline measures its ability to resist auto-ignition commonly referred to as pre-ignition or pinging. The diesel fuel cetane number, however is actually a measure of fuel ignition delay time period between the start of the injection of the fuel and the start of the combustion of the fuel (commonly known as ignition). Therefore, there should be a compromise between “octane number that wants to resist auto-ignition and cetane number that wants to support auto-ignition”.

The problem is how to get a working relationship between cetane number of a diesel engine and an octane number of a gasoline engine or vice versa with ignition delay and vehicle inter-convertion. There have been so many suggestions in literature on inter-convertibility of diesel to gasoline or vice visa with their attendant problems of adjustment on ignition, additive concentration, pressure and temperature of a compression cylinder. If a working relationship between cetane number, octane number and perhaps ignition delay are known, it will help in trying to understand what happens if one fuel engine converts to another type of fuel engine. The relationship between ignition delay, pressure and temperature during combustion will also be clear if a model is established to connect these parameters.

It is important to find a working relationship that certain engine combustion chambers obey between the conversions of the use of one type of fuel to the other. This will go a long way to alleviating the problem of engine knock and other knock associated problems that may be unforeseen in an engine that converts the use of one type of fuel to the other.

The objective of this work is to establish a working relationship between cetane number of diesel engine and octane number of a gasoline engine of a fuel convertible engine from the use of one fuel type to another and as it relate to an ignition delay. This work will also establish pressure, temperature relationship with ignition delay of an engine combustion chamber. When establish, it will go a long way to ease the understanding of the kinetics and thermodynamics of combustion chamber.

The scope of the work is to establish a working model relationship between the cetane number of a diesel engine and an octane number of a gasoline engine as they relate to ignition delay, on one hand, and thermodynamics and kinetics pressure, temperature relationship with ignition delay in an engine combustion chamber, on the other hand. This work do not include going into the intricatcy of the mechanics of combustion engines.

2. LITERATURE REVIEW

2.1 Cetane Number

Cetane number according to Werner (2007), is a measure of the quality of a diesel fuel or the ignition quality of a diesel engine fuel by comparison with various mixtures in which the alpha form of methylnaphthalene is given a standard value of 0 (zero) and cetane is given a standard value of 100.

According to Ulliman et al. (1994), cetane number measures the ignition quality of a diesel fuel. It is the percentage volume of cetane (n-hexadecane, Cetane Number = 100) in alpha methyl naphthalene (Cetane Number = 0), that provides specified standard of 13 degrees (crankshaft angle) ignition delay at the identical compression ratio to that of the fuel sample (Ulliman et al., 1994). These days, heptamethyl nonane – with a cetane number of 15 – is used in place of alpha methyl naphthalene because it is a more stable reference compound.

Cetane number is normally measured in special ASTM variable compression ratio test engine that is closely controlled with regard to temperatures (coolant 100ºC, intake air 65.6ºC), injection pressure (1500psi), injection timing 13 degrees BTDC, and speed (900rpm). The compression ratio is adjusted until combustion occurs at TDC (the ignition delay is 13 degrees). The test is then repeated with reference fuels with five cetane numbers difference, until two of them have compression ratios that bracket the sample. The cetane number is then determined by interpolation, and the higher the cetane number, the shorter the delay between injection and ignition.

Now, if the fuel is pure hydrocarbons (does not contain cetane number improving agents like alkyl or amyl nitrates) then the cetane number can be predicted fairly well using some physical properties, such as boiling point and aniline point. It's obvious from the above that the higher the cetane number (100 = normal alkane, 15 = iso-alkane), then the lower the octane number (100 = iso-alkane, 0 = normal alkane). This is because the desirable property of gasoline to prevent knock is the ability to resist auto ignition, whereas for diesel, the desirable property is to auto ignite. The octane number of normal alkanes decreases as carbon chain length increases, whereas the cetane number increases as the carbon chain length increases. Many other factors also affect the cetane number, and around 0.5 volume % of cetane number improvers will increase the cetane number by 10 units. Cetane number improvers can be alkyl nitrates, primary amyl nitrates, nitrites, or peroxides (Ziliang et al., 2000).

In general, aromatics and alcohols have low cetane numbers (that's why people using methanol in diesels convert it to dimethyl ether). One of the obvious effects of running on low cetane number fuel is the increase in engine noise. Typically engines are designed to use fuels with cetane numbers of 40-55, because below 38 a more rapid increase in ignition delay occurs. The significance of the cetane number increases with the speed of the engine, and large, low speed diesel engines often only specify viscosity, combustion and contaminant levels, as cetane number requirement of the engine is met by most distillate and residual fuels that have the appropriate properties. High speed diesel engines (as in cars and trucks) virtually all are designed to accept fuels around 50 cetane numbers, with higher numbers being a waste.

However, Cetane Number is only one important property of diesel fuels, with three of the others being also very important. Firstly, the viscosity is important because many injection systems rely on the lubricity of the fuel for lubrication. Secondly, the cold weather properties are important, remember that normal alkanes are desirable, but the desirable diesel fraction alkanes have melting points above 0ºC temperature, so special flow-enhancing additives and changes to the hydrocarbon profiles occur seasonally. That's why it's never a good idea to store diesel from summer for winter use, or harmattan for rainy season use. Thirdly, diesel in many countries has a legal minimum flash point (the minimum temperature it must attain to produce sufficient vapours to ignite when a flame is applied. In all cases it's usually well above ambient (60C+, kerosene is 37C+, whereas gasoline is typically below -30C), and anybody mixing a lower flash point fraction with diesel will usually void all insurance and warranties on the vehicle. The recent increase in blending fuels has resulted in significantly more frequent analyses of fuel tank contents from diesel vehicle fires (Baxleg and Rendel, 1931).

2.2 Octane Number

Octane number is a standard measure of the performance of an engine or aviation fuel (ASTM, 1988). The higher the octane number, the more compression the fuel can withstand before detonation (ignition). In broad terms, fuels with a higher octane rating are utilized in high performance gasoline engines that require compression ratios. In contrast, fuels with lower octane numbers (but higher cetane numbers) are ideal for diesel engines., because diesel engines (also referred to as compression-ignition engines) do not compress the fuel but rather compress only air and then inject the fuel into the air heated up by compression. Gasoline engines rely on ignition of air and fuel compressed together as a mixture without ignition, which is then ignited at the end of the compression stroke using spark plugs. Therefore, high compressibility of the fuel is of paramount interest for gasoline engines. Use of gasoline with lower octane numbers eventually leads to the problem of engine knocking.

Just as synonymous to cetane number, copious works have also been done on the concept of octane number. Taylor (1994) investigated the characteristics of combustion control with direct methanol injection in homogeneous charge compression ignition (HCCI) combustion over a wide operating range under several conditions including different compression ratios and three main fuels with different octane numbers. The operating range of HCCI combustion was limited by knocking at one extreme and misfire at the other. On the knocking side, they showed that moderate ethanol injection is effective at preventing knock. To extend the misfire limit, a lower octane number fuel yields a greater low-temperature heat release, increasing the temperature in the interval between the low- and high temperature oxidation, which prevents misfiring. Thus, they found that a combination of lower and compression ratio and lower octane number fuel assisted by a direct methanol injection can expand the operating load range envelope as the low-temperature oxidation can be controlled flexibly by varying the quantity of methanol injection with the operating condition. They concluded that the ignition suppression effect of methanol in HCCI combustion is much stronger than those of other fuels with a similar octane number (Challen and Barneseu, 1999).

In the same vein, an experimental study of partially premixed compression ignition combustion with low octane fuel was conducted by Ziliang et al., (2000) with low octane fuel in a single-cylinder engine. The effects of the external exhaust gas recirculation and intake boost on this partially premixed compression ignition combustion and emissions were investigated. During the experiments, a trade-off relationship between the NO_x and smoke emissions was observed in this partially premixed compression ignition combustion. However, heavy exhaust gas recirculation usage has the potential to decrease NO_x and soot emissions simultaneously at the expense of the fuel economy. They determined that at an increased intake port pressure, the maximum in-cylinder pressure increases, and the ignition timing of the high-temperature combustion is retarded. Also, the peak value of the low-temperature combustion was slightly depressed, the peak value of the high-temperature heat release decreases significantly, and the maximum value of the diffusing burn increases to some extent. More so, they concluded that compared to natural aspirated condition, that the partially premixed compression ignition combustion with intake boost has the capability of simultaneously reducing NO_x and soot emissions to ultra-low levels, that is, the intake boost could be an important strategy for the combustion and emission improvement in this advanced engine combustion mode.

Phuong et al. (2000), in a study" predict octane number" constructed a method to estimate the research octane number (RON) of different gasoline by using the results form gas chromatograph. This model has a standard error of 2.8 points, probably due to the assumption of linearity in octane blending. Very recently, Phuong et al. (2000) created an improved model form experiment data of 1471 gasoline. The analysis was conducted in other to determine the composition of each fuel.

Attempts to blend in the fuel tank should be carefully planned. One should not allow the tank to become empty, and then add 50% of lower octane, followed by 50% of higher octane. The fuels may not completely mix immediately, especially if there is a density difference. You may get a slug of low octane that causes severe knock. Tanks should be refilled when it is half full. In general the octane response will be linear for most hydrocarbon and oxygenated fuels eg 50:50 of 87 and 91 will give 89. Attempts to mix leaded high octane to unleaded high octane to obtain higher octane are useless for most commercial gasolines. The lead response of the unleaded fuel does not overcome the dilution effect, thus 50:50 of 96 leaded and 91 unleaded will give 94. Some blends of oxygenated fuels with ordinary gasoline can result in undesirable increases in volatility due to volatile azeotropes, and some oxygenates can have negative lead responses. The octane requirement of some engines is determined by the need to avoid run-on, not to avoid knock (ASTM, 1988).

2.3 Relationship between Cetane Number and Octane Number

Only a handful of studies exist on the relationship between cetane and octane numbers. Werner (2007) studied the relationship of cetane and octane numbers by expanding on the work conducted at the same laboratory in the middle 1960's. A total of 66 gasoline samples, which included commercial gasolines of the premium, regular, low-lead, and unleaded varieties, full boiling range reference fuel blends both conventionally leaded and unleaded, and samples meeting Federal Specification VV-G-001690 (Army-MR) and VV-G-76b, were evaluated for cetane number, motor and research octane number, hydrocarbon type, and lead content. They subjected the data to a regression analysis computer program from which correlations for octane-cetane numbers were developed by the researchers. The effects of other gasoline properties on these correlations were also investigated. They developed a satisfactory correlation of motor octane numbers with cetane numbers for gasolines in the 75- to 94-MON range was developed which has a standard error of estimate of ±1.71. The linear equation for this correlation differs from previous published ones due primarily to differences in the fuels used. It was observed that the research octane number-cetane number correlation with a standard error of estimate of ±1.09 appears to be much better than the motor octane number-cetane number correlation.

More so, the most significant relationship according to Taylor (1994) is that higher the cetane number (100 = normal alkane, 15 = iso-alkane), then the lower the octane number (100 = iso-alkane, 0 = normal alkane). According to him, this is because the desirable property of gasoline to prevent knock is the ability to resist autoignition, whereas for diesel, desirable property is to autoignite. The Octane number of normal alkanes decrease as the carbon chain length increases, whereas the cetane number increases as the carbon chain length increases (Taylor, 1994).

3. METHODOLOGY

3.1 DEVELOPMENT OF MODELS

3.1.1 Relationship between cetane and octane number

The change in an engine cetane number (CN) is always proportional to the natural logarithm of the change in the reciprocals of an engine Octane number (N).

$$\Delta C \propto \ln\left(\Delta {}^{1}/_{N}\right) \quad 3.1$$

i.e $$[C - C_0] \propto \ln\left({}^{1}/_{N} - {}^{1}/_{N_0}\right)$$

$$[C - C_0] = b \ln\left({}^{1}/_{N} - {}^{1}/_{N_0}\right) \quad 3.2$$

Rearranging equation 3.2 gives;

$$\ln\left({}^{1}/_{N} - {}^{1}/_{N_0}\right) = \frac{[C-C_0]}{b} \quad 3.3$$

Taking the antilogarithm of both sides of equation 3.3 and rearranging gives;

$$ {}^{1}/_{N} = e^{\left(\frac{C-C_0}{b}\right)} + {}^{1}/_{N_0} \quad 3.4$$

$$N = \frac{N_0}{1+N_0\, e^{\left(\frac{C-C_0}{b}\right)}} \quad 3.5a$$

or, octane number is partly directly (i) proportional to the square of cetane number (ii) proportional to the cetane number and (iii) a constant

i.e $$N = a_0C^2 + a_1C + a_2 \quad 3.5b$$

where N = octane number, and C = cetane number

3.1.2 Alternative relationship between cetane and ignition delay

Cetane number is partly proportional to the natural logarithms of ignition delay and partly a constant.

$$CN = a + b \ln \tau \quad 3.6$$

3.1.3 Relationship between ignition delay, % additive concentration, pressure or temperature

$$\tau = ae^{bx} + ce^{dx} \quad 3.7$$

where; τ = ignition delay, and x = % additive concentration, pressure or temperature

3.1.4 Relationship between octane number, cetane number and ignition delay

The relationship between octane number, cetane number and ignition delay can be express as;

$$Z = a_0 + a_1X + a_2Y + a_3XY + a_4X^2 + a_5Y^2 \quad 3.8$$

where; Z = τ = ignition delay, X = ON = octane number, Y = CN = cetane number

3.1.5 Relationship between percentage volume additive and increase in cetane number

The relationship between percentage volume additive (2-Ethylhexyl Nitrate) and increase in cetane number will assume the form of the model;

$$F(x) = U\exp(-B\exp(-kx)) \quad 3.9$$

or, $$F(x) = a_1X^3 + a_2X^2 + a_3X + a_4 \quad 3.10$$

where F(x) = % volume additive, X = cetane number

3.1.6 Relationship between ignition delay, % additive volume and pressure or temperature

The relationship between ignition delay, % additive volume, pressure or temperature is given as;

$$\tau = ae^{bx} + ce^{dx} \quad 3.11a$$

$$\tau = U\exp(-B\exp(-kx)) \quad 3.11b$$

where; τ = ignition delay, and x = % additive aditive, pressure or temperature

3.2 COLLECTION OF DATA

Parts of the data for validation of the models are obtained from experimentation and others from the experimental works of other researchers in the internet. This is because the experiment to determine the octane number is not only complicated, but will also require high class equipment.

3.2.1 Experimental set-up and procedure for the measurement of ignition delay and determination of pressure and temperature effects on ignition delay time of diesel fuel

Effect of pressure and temperature on Ignition Delay was determined using the Ignition Quality Tester (IQT). The Ignition Quality Tester comprises of a constant volume (0.213L) combustion chamber, pre-heated to the standard test temperature of approximately 828K via external electrical heater consisting of nine cartridge-type resistant heaters, a fuel injection system, an intake system, an exhaust system, a cooling system and a computer with a screen that is used to control the experiment, record and interpret data (fig 3.2). The charge air pressure and temperature are 145psi (10 bar) and 828K respectively. The IQT is a high temperature combustion device that simulates compression temperatures in diesel engines, but at a reduced air pressure (ASTM, 1988). The operational control parameters of the IQT allow data to be collected over a wide range of operating conditions (Ulliman, 1999).

To determine the pressure effect on Ignition delay, diesel fuel from the fuel reservoir was contacted with nitrogen from the nitrogen supply, the premixed fuel was then delivered to the constant volume combustion chamber by the help of a pneumatically driven mechanical fuel pump which was used to compress the fuel and deliver it to the combustion chamber via an inward opening single-hole pintle-type injector nozzle. The fuel pump temperature is approximately 308K before injection (Ziliang et al., 2000). The needle is spring-loaded with a screw and a lock nut for adjusting the nozzle opening pressure/release setting. The opening pressure on the injector was set to 145psi (10 bar), thus the fuel injection pressure by this arrangement was approximately 145psi during the main injection period. A fixed volume of fuel was injected (72mg for each injection event) into the combustion chamber. The mass of fuel injected was controlled by varying the thickness of the shim in the injection pump. The thermodynamic conditions in the combustion chamber are influenced by the charge pressure (combustion air), chamber temperature and fuel injection quantity (Taylor, 1994). Each injection event produces a single combustion cycle in which auto-ignition occurs. The temperature in the combustion chamber was kept constant at 828K by the help of the temperature control system of the IQT and Liquid to Air Heat Exchanger installed along the axis of the chamber. The chamber pressure decreases after the start of injection (SOI) due to evaporative cooling of the vaporising droplets injected. The pressure in the combustion chamber increases very rapidly once sustained combustion begins to occur (Taylor, 1994). Ignition delay was defined as the time between the start of injection (SOI) and the recovery of the combustion chamber pressure to 145psi (10 bar) [i.e. start of combustion (SOC)] as recorded by the aid of a computer (sensor) which traces the chamber pressure rise via the needle-lift and displaces it on a screen. The sequence was run for 32 injection cycles and the average ignition delay of the 32 cycles was taken after initial 15 pre-injection (warm-up) cycles to allow the chamber to attain thermal equilibrium. A liquid cooled piezo-electric pressure transducer, installed along the axis of the combustion chamber opposite to the nozzle, measures the chamber gas pressure before the start of injection (SOI) till the end of the test. The entire IQT test sequence requires about 17 minutes (Taylor and Michael, 2004).

The injection pressure was then changed and set to different test pressure values of 170psi (11.7bar), 217psi (15bar), 290psi (20bar), 363psi (25bar) and 435psi (30bar) for $0.08 \leq \phi \leq 0.25$ and the corresponding average ignition delay times for 32 experimental injections cycles (for each test pressure value) was taken and recorded. The chamber is purged with a constant stream of air after each combustion event and then refilled with pressurized air having an oxygen concentration of 20.9% (Taylor, 1994).

3.2.2 Experimental procedure for the measurement of cetane number, determination of the effect of cetane number improver [2-ethylhexyl nitrate (2-EHN)] on cetane number, and the effect of cetane number on ignition delay of diesel fuel

Cetane number, effect of cetane number improver, principally 2-ethylhxyl nitrate and the effect of cetane number on ignition delay was determined using the Ignition Quality Tester (IQT).

First, a sample of the test (base) fuel at 308K and 310 psi (21.4 bar) was charged into the IQT constant volume combustion chamber already preheated to the combustion temperature of 828K to determine the test (base) fuel cetane number (ASTM, 1988). The charge air temperature and pressure are 828K and 145psi (10 bar) respectively. A constant mass of fuel (72mg) was injected for each cycle. Auto ignition occurs inside the combustion chamber after the injection. The system was allowed to run for 32 injection cycles and the average time between the start of injection (SOI) and the recovery of the combustion chamber pressure to 310psi (21.4 bar) [i.e. start of combustion (SOC)] for the 32 injection cycles was taken as the ignition delay (ASTM, 1988). The measured average ignition delay for the 32 injection cycles was then used to determine the cetane number of the test fuel using an empirical inverse relationship of ignition delay according to ASTM D6890 test method.

Next, the test fuel was then separated and poured into four (4) 10L gallon samples, with each sample duly labelled. Then, 2-Ethylhexyl nitrate (2-EHN) of volumes 3ml (0.03%), 6ml (0.06%), 20ml (0.2%) and 30ml (0.3%) was pipetted into each of the four (4) 10L gallon samples of test diesel. The first sample consisting of a mixture of the test diesel and 0.03% 2-EHN was then injected into the constant volume combustion chamber of the IQT at 308K and 310 psi (21.4 bar). The charge air temperature and pressure was still maintained at 828K and 145psi (10 bar) respectively (Phuong, 2000). A constant mass of the sample fuel (72mg) was injected for each cycle. The average ignition delay of the sample fuel was determined after 32 injection cycles/sequence by measuring time between the start of injection (SOI) and the recovery of the combustion chamber pressure to 310psi (21.4 bar) [i.e. start of combustion (SOC)] for the 32 injection cycles. The ignition delay was then used to determine the cetane number of the first sample fuel using an empirical inverse relationship of ignition delay according to ASTM D6890 as before. The difference between the sample fuel derived cetane number and the test fuel derived cetane number was taken as the increase in cetane number (ASTM, 1988). The experimental procedure was repeated for other three (3) samples of 10L diesel fuels containing 6ml (0.06%), 20ml (0.2%) and 30ml (0.3%) 2-EHN.

Figure 3.1: Ignition Quality Tester (IQT) instrument

3.3 TABULATED INTERNET/LITERATURE VALUES

Table 3.1: Ignition delay versus octane number and cetane number for convertible fuel engine (Ziliang et al., 2000)

ON [X]	0	20	40	60	80	100	120	134
CN [Y]	58	50	43	33	20	5	-8	-20
τ_1[Z] (ms)	3.5	4.08	4.86	6.0	8.69	12.49	17.2	23.09

Table 3.2: Ignition delay versus pressure and temperature of an engine combustion chamber (Ziliang et al., 2000)

T (K) [X]	700	717	750	800	850	900
P_2 (atm) [Y]	9.15	10.5	12.9	22.8	24.9	26.5
τ_2 (ms) [Z]	2.65x 10^{-2}	1.5x1 0^{-2}	0.9x1 0^{-2}	5.13x 10^{-3}	5.0x1 0^{-3}	4.88x 10^{-3}

4. RESULTS AND DISCUSSION

4.1 RESULT PRESENTATION

The experimental results are as shown in tables 4.1 – 4.2 and figures 4.1 – 4.7 herein below.

Table 4.1: Experimental values of ignition delay versus pressure, at 828K

τ_2 (ms)	1.75x1 0^{-2}	1.25x1 0^{-2}	1.75x1 0^{-3}	5.25x1 0^{-3}	5.0x1 0^{-3}	4.7x1 0^{-3}
P_2 (atm)	10	11.7	15	20	25	30

Table 4.2a: Experimental values of cetane improver (%volume), ignition delay, cetane number and increase in cetane number

T = 828K, P = 310psi (21.4bar)

S/N	Cetane Improver (2-EHN) %vol.	τ_2 (ms)	Cetane Number	Increase in Cetane Number
1	0.00	5.19	40.40	0.00
2	0.03	4.82	43.20	2.80
3	0.06	4.57	45.30	4.90
4	0.20	4.35	47.40	7.00
5	0.30	4.23	48.60	8.20

Table 4.2b: Experimental values of ignition delay versus temperature, at 101.5psi

τ_2 (ms)	282.0	179.5	145.3	60.8	31.2	18.1	11.9	7.2
T (K)	450	650	700	740	806	847	900	957
1000/T(K^{-1})	2.20	1.53	1.42	1.35	1.24	1.18	1.10	1.04

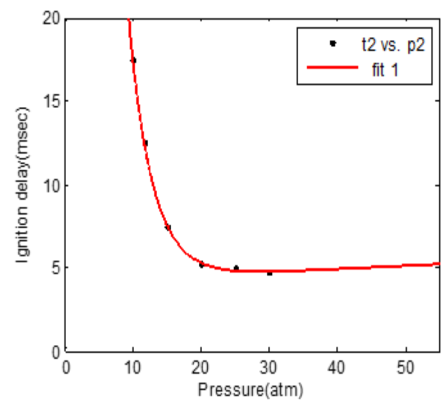

Figure 4.1: Ignition delay versus pressure in IQT diesel combustion engine (chamber) at 828K, and constant mass of fuel. Each data point is a single injection event (table 4.1, eqn 3.7).

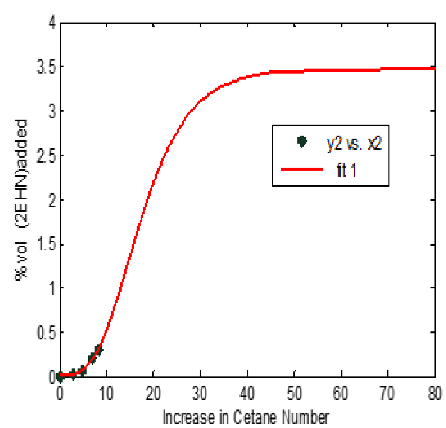

Figure 4.2a: Cetane improver (%vol.) versus increase in cetane number in IQT diesel combustion engine (chamber) at 310psi and 828K, constant mass of fuel. Each data point is a single injection event (table 4.2a, eqn 3.9).

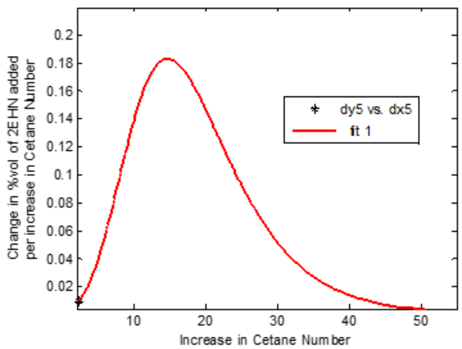

Figure 4.2b: Change in % volume of 2EHN added per increase in cetane number versus increase in cetane number.

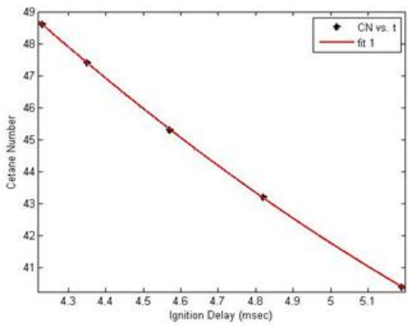

Figure 4.3: Cetane number versus ignition delay in IQT diesel combustion engine (chamber) at 310psi and 828K, constant mass of fuel. Each data point is a single injection event (table 4.2a, eqn 3.9).

Table 4.3: Coefficients and goodness of fit, for fig 4.1 (eqn 3.7)

95% Coefficient Bound	Goodness of Fit
a = 0.15 b= -0.2498 c = 0.004089 d = 0.003512	SSE = 2.342e-007 R^2 = 0.9982 R^2 Adj.= 0.993 RMSE = 0.000484

Table 4.4: Coefficients and goodness of fit, for fig 4.2a (eqn 3.9)

95% Coefficient Bound	Goodness of Fit
U = 3.469 B = 7.741 K = 0.1408	SSE = 0.0003137 R^2 = 0.9952 R^2 Adj.= 0.9903 RMSE = 0.01252

Table 4.5: Coefficients and goodness of fit, for fig 4.3 (eqn 3.9)

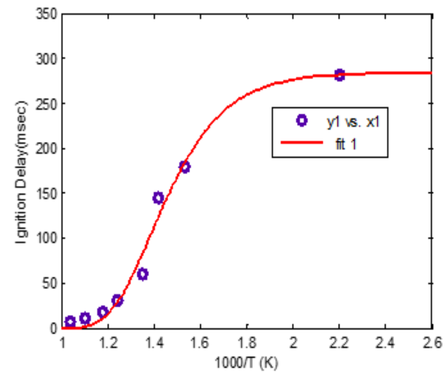

Figure 4.4a: Ignition delay versus temperature in IQT diesel combustion engine (chamber) at 101.5psi and (7bar), and constant mass of fuel. Each data point is a single injection event (table 4.2b).

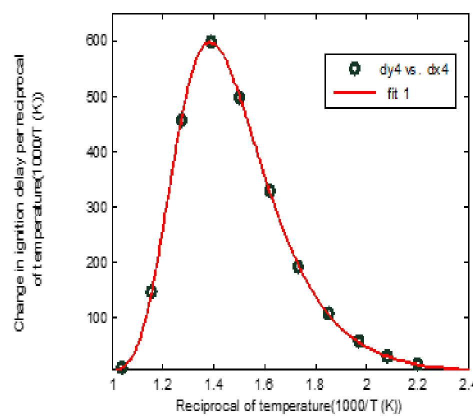

Figure 4.4b: Change in ignition delay per reciprocal of temperature versus reciprocal of temperature.

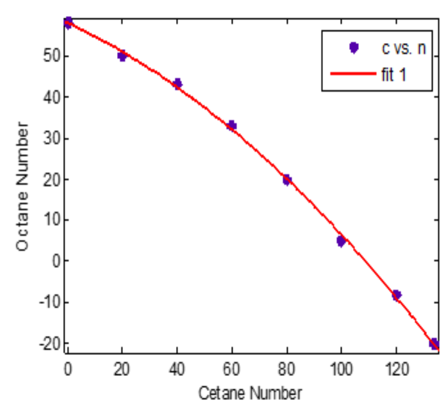

Figure 4.5: Octane number versus cetane number of a convertible fuel engine (table 3.1, eqn 3.5b)

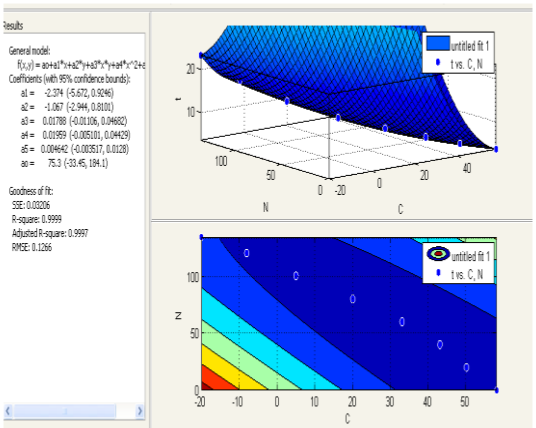

Figure 4.6: Ignition delay versus octane number and cetane number of a convertible engine (table 3.1)

Table 4.6: Coefficients and goodness of fit, for fig 4.4a (eqn 3.11)

95% Coefficient Bound	Goodness of Fit
U = 2713 B = 285.1 K = 5.703	SSE = 1148 R^2 = 0.9837 R^2 Adj.= 0.9772 RMSE = 15.15

Table 4.7: Coefficients and goodness of fit, for fig 4.5 (eqn 3.5b)

95% Coefficient Bound	Goodness of Fit
a_1 = -0.3076 a_2 = 57.88 a_0 = -0.002053	SSE = 5.214 R^2 = 0.9991 R^2 Adj.= 0.9987 RMSE = 1.021

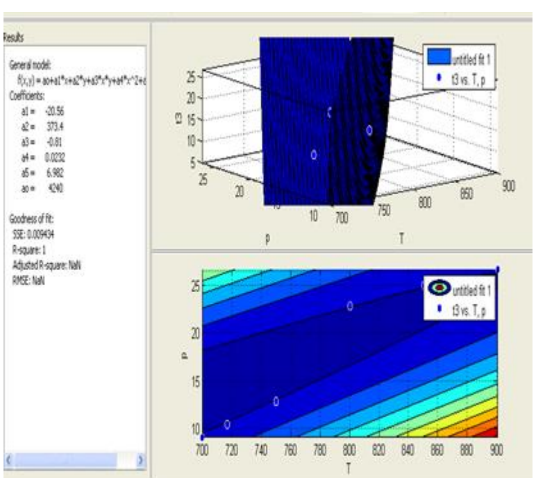

Figure 4.7: Ignition delay versus pressure and temperature of engine combustion chamber (table 3.2).

4.2 DISCUSSIONS

Figure 4.1 (table 4.1) shows the plot of ignition delay versus pressure at 828K. Ignition delay decreases with corresponding increase in pressure from the profile. However, at certain pressure level, (about 20atm) the pressure fall rate decreases drastically and continues ad infinitum. This implies that at high pressures, pressure seldom has significant effect on the ignition delay decreases.

Figure 4.2a (table 4.2a) shows the effect of additive, (2-EHN, used to raise or improve cetane number). The curve shows a gradual increase in cetane number with percentage volume increase in 2-EHN. From the profile, 2-EHN gives a direct function with cetane number. This implies that the higher the volume of 2-EHN, the higher the increase in cetane number and vice versa. However, this increase in cetane number tends to tapper out asymptotically at certain percentage volume concentration of 2-EHN. This means that beyond certain percentage additive volume, it tends to attain a limiting value and stops increasing no matter the increase in cetane number.

The curve (figure 4.2a) which is synonymous to an initial semi-parabola depicts a gradual increase in cetane number with percentage volume increase in 2-EHN. Between 0.0 to 0.06% 2-EHN, the curve rises steadily with gentle slope which then culminates to geometric increase between 0.06 to 0.30% with steep slope. At higher increases in cetane number the curve tappers out asymptotically and tends to be parallel to x-axis.

In figure 4.2b, which is a numerical differential plot of figure 4.2a, is a dumb bell of peak f(14.6) = 0.183135 i.e the optimum of 14.6 cetane number increase gives an optimum of 0.183135 %volume of additives.

Figure 4.3 (table 4.2a) shows cetane number-ignition delay relationship. The figure shows that Ignition Delay decreases with increase in cetane number and vice versa. Thus, at higher cetane number values, shorter ignition delays are observed from the profile. Higher cetane numbers from the profile corresponds to shorter ignition delays, thus, availing more time for the fuel combustion process to be accomplished efficiently. More so, the profile portrays ignition delay as an inverse profile of cetane number of a diesel fuel.

In figure 4.4a, ignition decreases as combustion temperature increases and vice versa, which invariably portrays ignition delay as an inverse function of combustion temperature. Shortest ignition delay (7.2ms) from the profile is observed at the zenith combustion temperature of 957K. this can be attributed to that fact that inside the combustion chamber of the IQT, though evaporative cooling of the fuel droplets occurs, (which gives rise to fall in temperature as well subsequent chamber pressure decreases at start of injection and/or ignition delay), but at higher temperature, the high temperature inside the chamber attenuates evaporative cooling effect, thus, giving rise to shorter ignition delays. From combustion temperature of

806K down, the curve rises geometrically, depicting a rapid increase in ignition delay as temperature plunges arithmetically and vice versa. The profile thus, depicts a strong ignition delay dependence on temperature.

In figure 4.4b, which is also a numerical differential plot of figure 4.4.a, is a dumb bell profile of peak f(1000/4) = f(1.388) = 598.16 i.e the optimum of T = 1000/1.388 = 720K, gives an optimum of 598msec of ignition delay.

In the same vein, figure 4.5 (table 3.1) gives the relationship between octane number and cetane number of a convertible engine. The profile which is synonymous to a trajectory vividly shows that octane number of gasoline fuels is an inverse function of the corresponding cetane number. This implies that the higher the octane number, the lesser the cetane number value and vice versa. Thus, a gasoline engine operating on a high octane number fuel, if converted to a diesel engine, operates on a diesel fuel with a low cetane number depending on the choice of fuel used. From the cursor contour of the 3-D plot of figure 4.6, cetane and octane number shoe inverse relation while the cursor contour of the 3-D plot of figure 4.7 show that pressure and temperature are in proportional relation.

5. CONCLUSION AND RECOMMENDATIONS

5.1 CONCLUSION

This work successfully modeled and validated the relationship between octane number and cetane number for conversion from diesel to petrol engine and vice versa. The Ignition Quality Tester (IQT) was used to carry out combustion experimental work on diesel fuel involving Ignition delay - temperature relationship as well as ignition delay - pressure relationship. The same was used to determine cetane number - ignition delay, %volume additive - increase in cetane number and octane number - cetane number relationships. Tests were conducted at constant pressure and temperatures of 145psi and 828K respectively. Experimental data were curve-fitted at R^2 of 0.9982%, 0.9952%, 0.9954%, 0.9937% and 0.9991% for ignition delay - pressure, %volume 2-EHN additive - increase in cetane number, cetane number - ignition delay, ignition delay - temperature, and octane number -cetane number experiments respectively. The experimental data agree very well with derived models and in real life. Model validation accuracy for the combustion relating to octane-cetane relationship gives R^2 value of 0.9991 which affirms that experimental data agree well with the derived model. The work can be utilized in automobile industry to ascertain the equivalence of converting from one fuel to the other vis-à-vis octane and cetanes based fuels and also correlate variable parameters in fuel combustion as the case may be.

5.2 RECOMMENDATIONS

More research work need to be done, on the relationship between octane and cetane number with much emphasis on the intricacies of the mechanics of combustion engine.

REFERENCES

[1] ASTM (1998). American Society for Testing and Material. Annual Book of ASTM Standards. Vol 5,04, Test methods for Rating Motor, Diesel and Aviation Fuel, ASTM, Easton, Maryland.

[2] Brewster B. and Kerly R.V. (1963). "Automotive Fuels & Combustion Problems," presented at SAE National West Coast Meeting, Seattle, Washington.

[3] Baxleg C.H. and Rendel T.B. (1931). "Report and the volunteer Group for Compression Ignition Fuel Research.

[4] Boerlarge G.D. and Broeze J.J. (1932). "Ignition Quantity of Diesel Fuels as Expressed in Catene Numbers" S.A.E Journal. July. pp. 283-293.

[5] Challen B. and Barneseu R. (1999). "Diesel Engine Reference Book", Society of Automotive Engineers. Bath pres, England.

[6] Phuong T.M., Do S. and Daniel E.R. (2000). "A catalylic Strategies for improving specific fuel properties."

[7] Ryan T.W., Callahan T.J. (2009). "Gas temperature during compression in motored and fired diesel engines". SAE Trans Vol 70: 136-145.

[8] Taylor J.D. and Michael J. (2004). "Compandium of Experimental Cetane Number Data". Golden Colorado: National Renewable Energy Laboratoy, 48.

[9] Taylor C.F. (1994). "The Internal Combustion Engine in Theory and Practice". Vol. 2. Combustion, Fuel, Material, Design, MIT Press Cambridge.

[10] Urban C.M. and Gray J.T. (1968). "An Investigation of Methods for Determining Cetane Numbers of Low Ignition Quantity Fuels, "presented at SAE Mid-Year Meeting, Detroit, Michigan.

[11] Ullman T.L., Spreen K.B. and Mason R.L. (1994). "Effects of Cetane Number, Cetane Improver, Aromatics and Oxygenate on 1994 Heavy-Duty Diesel Engine Emissions", Society of Automotive Engineers Inc., SAE 941020.

[12] Werner D., Arno R.Z., Andrea S. and Klaus R. (2007). "Automotive Fuel" in Ullmann's Encyclpediaof Industrial Chemistry, Wiley-VCH.

[13] Ziliang Z., Tamer B. and Vaieim H. (2000). Investigation of Physical & Chemical Delay Periods of Different Fuels in the Ignition Quality Tester. Doctoral Dissertation: Wayne University.