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Effect of Cetane Improver on Autoignition Characteristics of Low Cetane Sasol IPK Using Ignition Quality Tester (IQT)

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ABSTRACT

This paper investigates the effect of a cetane improver on the autoignition characteristics of Sasol IPK in the combustion chamber of the Ignition Quality Tester (IQT). The fuel tested was Sasol IPK with a Derived Cetane Number (DCN) of 31, treated with different percentages of Lubrizol 8090 cetane improver ranging from 0.1% to 0.4%. Tests were conducted under steady state conditions at a constant charging pressure of 21 bar. The charge air temperature before fuel injection varied from 778 to 848 K. Accordingly, all the tests were conducted under a constant charge density. The rate of heat release was calculated and analyzed in details, particularly during the autoignition period.

In addition, the physical and chemical delay periods were determined by comparing the results of two tests. The first was conducted with fuel injection into air according to ASTM standards where combustion occurred. In the second test, the fuel was injected into the chamber charged with nitrogen. The physical delay is defined as the period of time from start of injection (SOI) to point of inflection (POI), and the chemical delay is defined as the period of time from POI to start of combustion (SOC). Both the physical and chemical delay periods were determined under different charge temperatures. The cetane improver was found to have an effect only on the chemical ID period. In addition, the effect of the cetane improver on the apparent activation energy of the global combustion reactions was determined. The results showed a linear drop in the apparent activation energy with the increase in the percentage of the cetane improver. Moreover, the low temperature (LT) regimes were investigated and found to be presented in base fuel, as well as cetane improver treated fuels.

INTRODUCTION

The ignition quality of the fuel has a major impact on the autoignition, combustion, fuel economy, performance and emissions of compression ignition diesel engines. The ignition quality of a fuel is rated by its cetane number (CN) measured in a Cooperative Fuel Research (CFR) engine according to ASTM D613 [1] or by its derived cetane number (DCN) measured in the Ignition Quality Tester (IQT) according to ASTM D6890 [2]. A higher CN implies better compression-ignition quality of the fuel, which produces shorter ignition delay (ID). A lower CN fuel produces longer ID, higher rates of pressure rise, pre-mixed burn fraction, and peak pressure, which result in unacceptable noise and vibration, and high mechanical and thermal stresses.

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The ignition quality of a fuel can be improved by adding very small amounts of an additive such as 2-ethylhexyl nitrate (2-EHN), a widely used cetane improver available in the market. Studies have shown that HC, CO, and NOx emissions decrease with the increase in CN [3-6]. However, there was no significant improvement in engine performance, reported by different researchers, when the CN was above a certain value [3,4]. Also, the effect of the cetane improver on autoignition was not uniform for different fuels during different engine operation conditions such as intake temperature, engine load, injection timing, etc [7-9]. Ghosh indicated that the degree of CN improvement was correlated to the quality of the original fuel, although the cetane improver enhances the initiation reactions, which accelerates the overall autoignition process [8]. Nuszkowski reported that the rate of heat release (RHR) is affected by the cetane additive at low load engine running conditions, resulting in the reduction in NOx emissions, but producing more NOx at high loads [7].

Few studies examined the effect of 2-ethylhexyl nitrate on the autoignition process [10,11], which is very slow for some alternate fuels [12,13], particularly when they exhibit the low-temperature combustion (LTC) regime [12-14]. The aim of this work is to investigate the effect of treating Sasol IPK with different percentages of 2-EHN on the autoignition process. The properties of Sasol IPK and the cetane improver are given in Appendix B.

EXPERIMENTAL SETUP

The experiments were conducted in the Ignition Quality Tester (IQT) [2] which is widely used to measure the DCN of fuels for diesel engines. Also, DCN is considered as one of the critical properties in the investigation of surrogates for aviation fuels [15-17]. The fuel sample is filtered prior to the test by using a syringe fitted with a disposable 5 µm filter and injected into pre-heated, temperature-controlled air. A complete sequence comprises 15 preliminary tests followed by 32 tests. The values for the ID of the last 32 tests are averaged to obtain the result. This test method covers ID periods that range from 3.1 to 6.5 ms, which correspond to 64 DCN and 33 DCN, respectively. The following equation is used to calculate DCN from the measured ID.

$$\mathrm{DCN} = 4.46 + (186.6/\mathrm{ID}) \quad (1)$$

For fuels that have ID shorter than 3.1 ms or longer than 6.5 ms, DCN can be calculated with less precision from Eqn. 2.

$$\mathrm{DCN} = 83.99 \times (\mathrm{ID} - 1.512)^{-0.658} + 3.547 \quad (2)$$

The IQT test is simpler than the CFR engine test because it requires a small sample of approximately 100 mL and the test takes approximately 20 min on a fit-for-use instrument [2,18]. In addition, the IQT test has higher repeatability and reproducibility compared to the CFR engine method [19,20], as shown in Appendix A. Furthermore, the IQT test is fully automated and can be run with minimal operator intervention.

The IQT is a bench-scale device, comprised of a constant volume combustion chamber with external electrical heating elements, a fuel injection system, an intake system, an exhaust system, a data acquisition system, and a cooling system. The combustion chamber is a cavity along a central axis of the body, with a volume of 0.213±0.002L, which is pre-heated to the standard test temperature of about 828 K by nine cartridge-type resistance heaters. The charge air pressure and temperature are 2.137±0.007 MPa and 818 ± 30 K respectively [2]. The IQT is a high temperature combustion device that simulates compression temperatures in diesel engines, but at a lower air pressure.

A pneumatically driven mechanical fuel pump is used to compress the fuel and deliver it into the chamber through an inward opening single-hole pintle-type injector nozzle. The needle is spring-loaded with a screw and a lock nut for adjusting the nozzle opening pressure/release setting [21]. The air pressure of the fuel pump actuator is 1.21±0.03 MPa. The fuel injection pressure is approximately 22.5 MPa during the main injection period. A fixed volume of fuel is injected. For n-heptane, the amount of fuel injected is 72±7 mg for each injection event [2,22]. 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 until the end of the test.

The IQT calibration procedure includes two reference fuels: n-heptane of DCN 53, with a minimum purity of 99.5% on the volume basis, and methylcyclohexane of DCN 23 [23], with a minimum purity of 99.0% on the volume basis. The average of three acceptable ID results of heptane is required to be within 3.78±0.01 ms, with no individual results below 3.72 or above 3.84 ms. The average of two acceptable ID results of methylcyclohexane is required to be within 10.4±0.5 ms, with no individual results below 9.8 or above 11.0 ms. If any of the results are outside the specified range, the system diagnostic procedures should be used to determine the problem and a new calibration is performed [2,18].

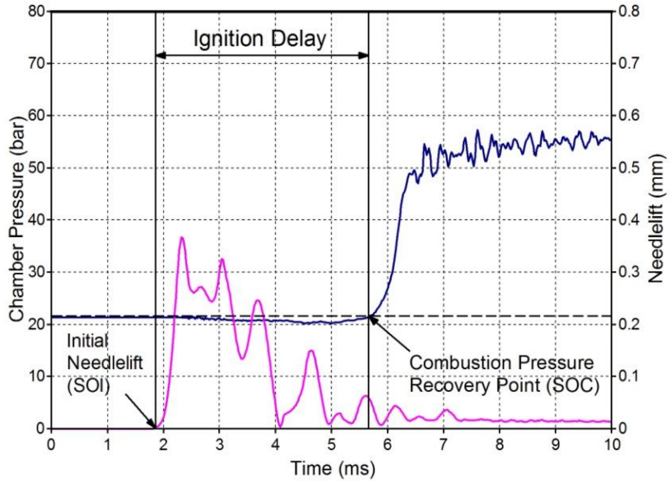


Figure 1 – A sample of traces for the needlelift and chamber pressure depicting the definition of IQT ignition delay time

The IQT equipment was utilized in the present investigation as a platform to investigate the physical and chemical processes that lead to the autoignition of different fuels under well-controlled charge pressure and different temperatures. There are many definitions of the ignition delay period in the literature. All researchers agree on the start of injection (SOI) as the start of ID. However, several criteria have been used to define the end of ID or the start of combustion (SOC) [24-32]. In the current investigation, the definition of ID specified in ASTM D6890 [2] was used as shown in Figure 1. It is the time elapsed from the SOI to the SOC. SOC in ASTM D6890 is defined as the time when the pressure in the chamber reaches 138 kPa above the initial chamber pressure. This point is considered to be the "combustion recovery point" [29,33-35].

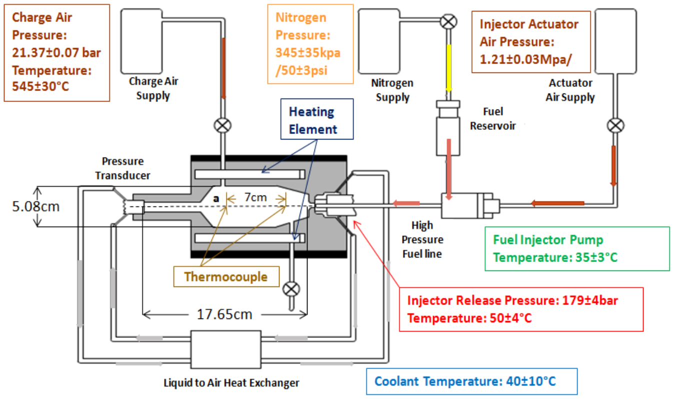


Figure 2 – Schematic of the Ignition Quality Tester setup at Wayne State University (WSU)

It should be noted that the maximum value of 0.4 mm for the needlelift (N.L) shown in all the figures in this paper are the print out of an earlier version of the IQT, purchased in 2007. The vendor Advanced Engine Technology (AET) corrected the lift to 0.8 mm in recent IQT software. There are no errors in the data for the ID in this paper, since the SOI does not depend on the maximum value of N.L.

A schematic of IQT along with a list of parameters and running conditions are given in Figure 2. There are two thermocouples inside combustion chamber along the axial direction. The first thermocouple measures the charge temperature close by the injector nozzle, the second thermocouple is 7 cm downstream from the first one. The temperature gradient increases approximately 40 °C from the first to the second thermocouple [22,35]. The local area where combustion starts in the IQT is close to the pressure transducer [35]. In order to capture the changing in temperature during the autoignition process, the thermocouple at position "a" was replaced with Omega K-type fast response 0.002" diameter junction. The thermocouple is connected to a compensation circuit with an amplifier module (Analog Device 5B40).

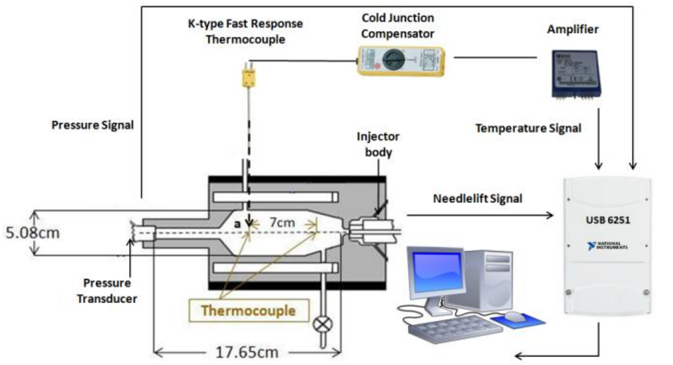


Figure 3 – Schematic of the additional DAQ system (based on reference [35])

An additional National Instrument (NI) high-speed multifunction data acquisition (DAQ) system was connected to the standard IQT system, in order to expand the capability of obtaining data, as shown in Figure 3. The N.L, pressure and temperature signals were simultaneously measured at a sampling rate of 1.25 MS/s. All the safety features were controlled by the standard IQT system.

SIMULATION MODEL

STAR-CD, a 3D CFD package coupled with DARS-CFD, is applied to simulate the behavior of the fuel spray in the IQT. Pro-star, sub-software of STAR-CD, is used to setup model parameters such as fuel injection, atomization, droplet, combustion, and etc. DARS-CFD performs calculations based on the chemical kinetics mechanism of n-heptane.

A combustion chamber is defined by a cylindrical coordinate system. The mesh consisting 38262 cells is created. Moreover, the calculation step size of 0.005 ms is set throughout the evaporation and combustion events to achieve higher accuracy.

The model assumes a Lagrangian approach to define spray-droplet behavior. The software code considers droplet trajectories, droplet break-up, collision and coalescence, wall interaction, wall heat transfer, and droplet evaporation. Reitz-Diwakar's [36] model is used for droplet break-up. Bai's [36] model is used for droplet wall interaction, including droplets adhesion, spread, rebound, and splash. Huh's [36] model is used for spray atomization calculations. Reynold Average Navier-Storkes (RANS) [36] model is used for turbulence calculation.

Pintle type nozzle is used in the model, in order to reproduce the conditions in the IQT. The reduced heptane model, used in the simulation, includes 35 species and 145 reactions [37].

RESULTS AND DISCUSSIONS

Effect of cetane improver on DCN

The ignition delay was measured for Sasol IPK, referred to as (S), Sasol IPK treated with 0.1% (volume basis) cetane improver, referred to as (ST0.1), Sasol IPK with 0.2% cetane improver, referred to as (ST0.2) and Sasol IPK with 0.4% cetane improver, referred to as (ST0.4) and their DCNs were calculated. The DCN for Sasol IPK was calculated by using Eqn. 2 as explained in the previous section because its ID was longer than 6.5 milliseconds. The DCNs for the treated fuel were calculated by Eqn. 1. The values for the DCN and the ID period for the (S) and (STs) are given in Table 1. It shows the ID was reduced, from 6.94 ms for (S) to 5.04 ms for (ST0.4); a reduction of 27%. The corresponding increase in DCN is 10.4 units. It should be noted that the increase in DCN is not linear with the percentage of additive. Figure 4 shows the increase in the DCN of the fuel with different percentages of the additive. The blue solid curve represents (S), and the red dash is for ultra low sulfur diesel (ULSD), which is a reference fuel, and the black dot is for the average increase in DCN of general fuels, reported by the additive manufacturer [38]. The sharpest increase in DCN is gained by adding the first couple droplets of the additive. The gain in DCN decreases continuously as the percentage of additive increases. Figure 4 shows also a higher rise in the DCN of (S) and (STs) over the average fuels [38]. It indicates that Sasol IPK is a high response fuel to Lubrizol 8090 [39], similar to ULSD. Further, it is noted that the rise in DCN of ULSD is slightly higher than Sasol IPK. This indicates that the original fuel with a higher DCN gets more benefits from the cetane improver than the one with a lower DCN [10]. It should be noted that the response of a base fuel to the additive is different than its response if it is treated. In the latter, the rate of increase in DCN reduces with the increase in percentage of the additive. The reason behind this difference in the response of base and treated fuels is not clear at the present time.

Table 1 –IQT DCN for (S) and (STs)

Fuel	IQT ID	IQT DCN	DCN Std Dev
(S)	6.94	31.1	0.58
(ST0.1)	5.58	37.9	0.51
(ST0.2)	5.33	39.4	0.61
(ST0.4)	5.04	41.5	0.53
ULSD	4.953	42.13	0.57
(ULSD0.1)	4.229	48.58	0.99
(ULSD0.2)	4.037	50.69	1.01
(ULSD0.4)	3.808	53.63	1.19

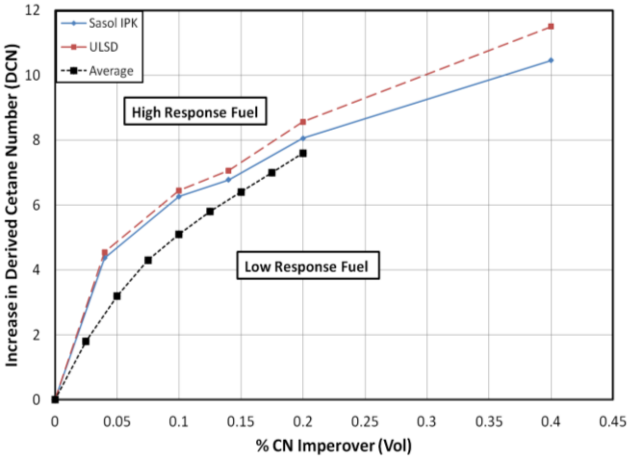


Figure 4 – Cetane improver typical treat rate response for Sasol IPK

Effect of cetane improver on autoignition

The time histories of the gas pressure, N.L, gas mass average temperature and rate of heat release (RHR) are given in Figure 5 for the (S) and (STs). The figure shows that, for all the fuels, SOI occurs at 2 ms, and the main injection process is completed in about 2 ms before the rise in pressure due to autoignition and combustion. As expected, (ST0.4) has the shortest ID and produces the lowest peak pressure and RHR. Since the volatility of the original fuel does not change with the additive percentage, the premixed combustion fraction and corresponding rise in pressure are expected to be proportional to the length of the ID as shown in Figure 6 and Table 2, compared with ULSD data [40].

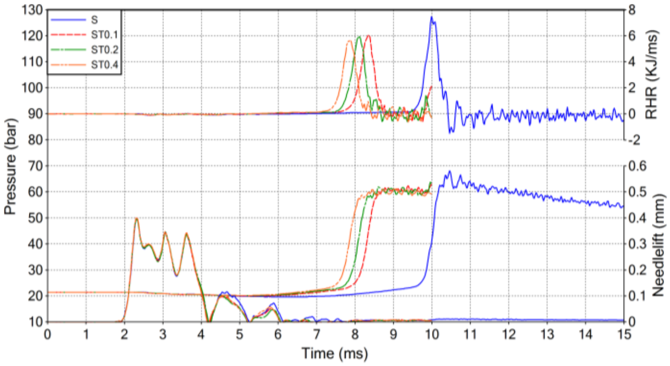


Figure 5 – Needlelift, pressure, RHR traces for different fuels at temperature 818K

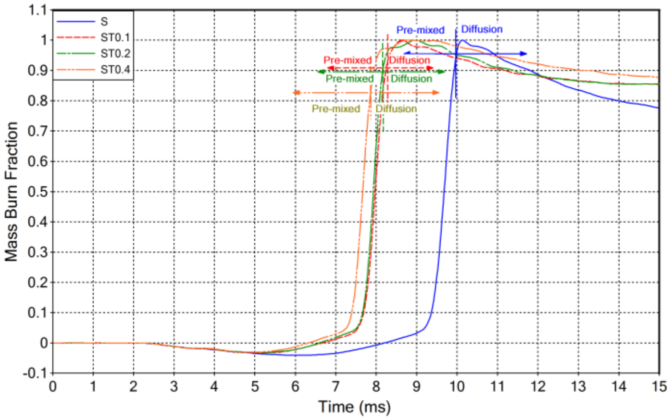


Figure 6 – Mass burn fraction for (S) and (STs) at temperature 818K

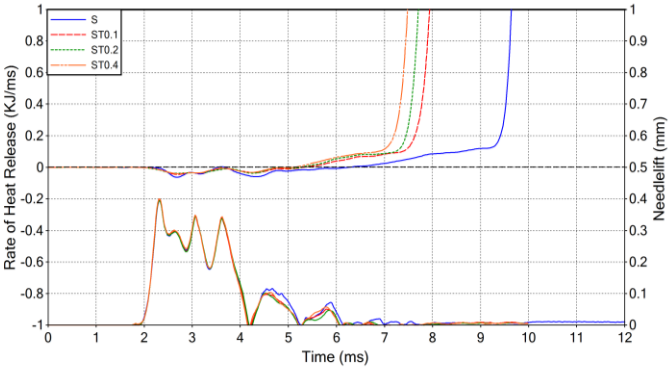


Figure 7 – Zoomed rate of heat release for different fuels at temperature 818 K

Figure 7 shows the zoomed RHR for (S) and (STs) at an air temperature of 818 K along with the N.L profile. It can be observed that after the end of the injection event there is a drop in RHR. This drop is mainly caused by the heat transferred from the air to the fuel for liquid heating, evaporation, vapor superheating and endothermic reactions. The oscillations in the traces are caused by the needle motion frequency [40]. The drop in RHR is followed by a gradual increase in the RHR to a plateau, followed by a sharp rise indicative of the start of exothermic reactions and the sharp rise in temperature. Figure 7 shows that all the fuels experienced the low-temperature plateau, with and without the additives. However, the period of the LT plateau decreased with additives. This suggests that the additive accelerates initiation reactions as well as exothermic high temperature reactions.

Table 2 – Energy Release of four fuels at temperature 818 K

Fuel	Pre-mixed (kJ)	Diffusion (kJ)	Pre-mixed fraction
(S)	2.7904	0.1393	95.25%
(ST0.1)	2.4944	0.2228	91.80%
(ST0.2)	2.4076	0.2686	89.96%
(ST0.4)	2.1626	0.4374	83.17%
ULSD	2.2506	0.6582	77.37%

Effect of cetane improver on physical and chemical processes

Effect of cetane improver on physical processes

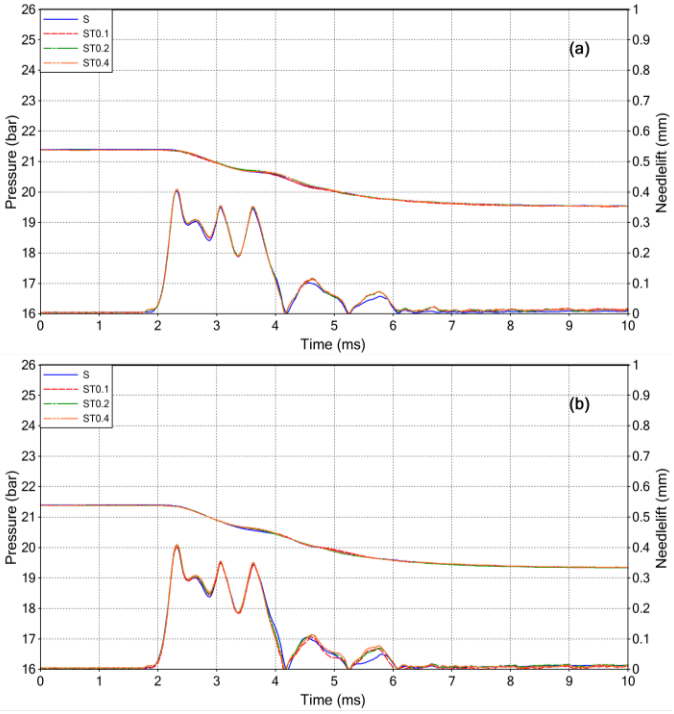
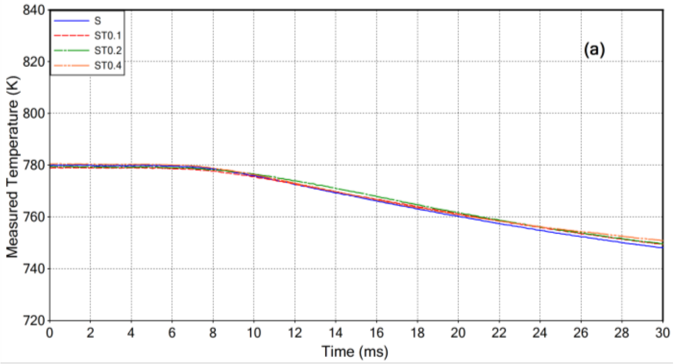


Figure 8a – Pressure and needlelift traces in nitrogen charge for (S) and (STs) at 778K
Figure 8b – Pressure and needlelift traces in nitrogen charge for (S) and (STs) at 848K

In order to investigate the effect of a cetane improver on physical processes, the fuels were injected into a nitrogen charge where the chemical processes are absent, except for the endothermic fuel dissociation processes. It should be noted that the drop in the RHR due to endothermic dissociation reactions has been reported to be insignificant if compared with the drop due to the physical processes in the IQT [40].

Figure 8 shows the time history of the pressure and N.L for (S) and (STs) injected into a nitrogen charge at two charge temperatures of 778K and 848 K. No difference is observed in all the traces for all the fuels.

Figure 9 shows the measured temperature profiles for (S) and (STs) injected into nitrogen. These temperatures were measured by the local thermocouple as shown in Figure 2. It is observed that the temperature profiles do not show any variations due to the additive at the two charge temperatures. Also, there is a delay in the start of the drop in temperature, compared to the start of the drop in pressure. This can be explained by the fact that the thermocouple measures a local temperature, while the pressure measures a global phenomenon.



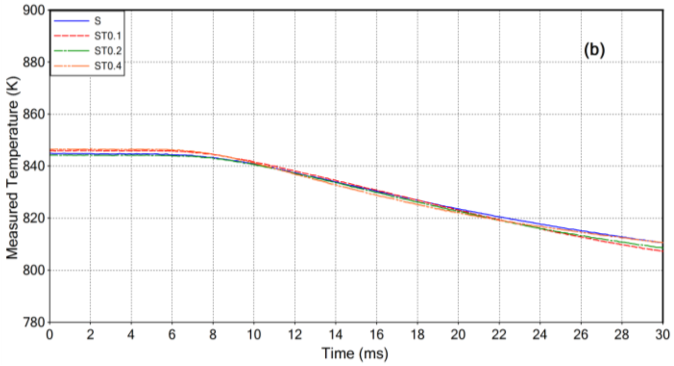


Figure 9a – Measured temperature traces in nitrogen charge for the (S) and (STs) at 778K

Figure 9b – Measured temperature traces in nitrogen charge for the (S) and (STs) at 848K

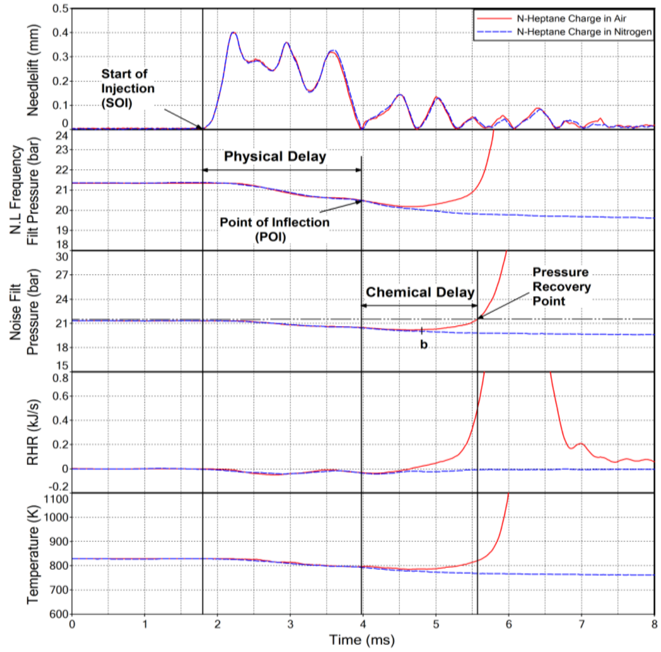


Figure 10 – Needlelift, pressure, RHR and temperature traces for fuel injection into air and into nitrogen

Effect of cetane improver on chemical processes at different charge temperatures

Figure 10 shows traces for the N.L, gas pressure, RHR and gas temperature with fuel injection into air and into nitrogen. The trace for injection in nitrogen continues to drop, indicating a continuation of liquid evaporation and endothermic reactions. The trace for injection in air changes its slope, indicating the start of active exothermic reactions. It should be noted that chemical reactions start immediately after fuel is injected. However, the rate of exothermic reactions is very slow that it could not cause a detectable deviation in the pressure and RHR traces, from that with nitrogen. This has been validated from the results of a computer simulation model of the gas pressure in the IQT, as shown in Figure 11. The blue trace is for the fuel injected into air with combustion. And the red trace is for the fuel injected into air without combustion. The point of separation between the two traces is defined as the point of inflection (POI), which determines the start of active exothermic reactions or the end of the physical delay period. Therefore, the physical delay is defined as the period of time from SOI to POI, and the chemical delay is defined as the period of time from POI to SOC as shown in Figure 10.

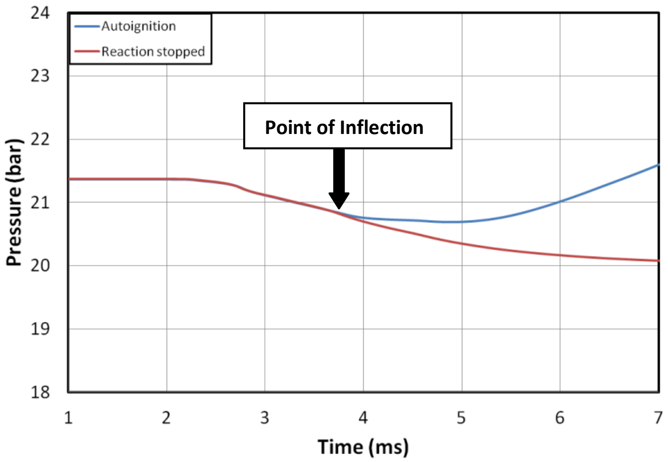


Figure 11 – 3D CFD simulation results of pressure traces in the IQT for fuel injection into air with and without combustion

A series of tests were conducted at different charge temperature between 778 and 848 K by controlling the chamber skin temperature. All the tests were conducted at a constant charge pressure of 21.37±0.07 bar (310±1 psi). The traces were analyzed, and the physical and chemical delays were determined for the (S) and (STs) at different charge temperatures. The results are given in Table 3 and plotted in Figure 12 versus the mean integrated temperature during the chemical ignition delay period, rather than the temperature at the SOI. The chemical ignition delay decreased with the increase in the percentage of the cetane improver. The decrease in the chemical delay becomes less at higher temperatures. These results also indicate that the effect of a cetane improver is more significant at low-temperatures [11].

Table 3 – Physical and chemical delay for four fuels at different temperature

	(S)		(ST0.1)		(ST0.2)		(ST0.4)	
Test T (K)	**Phy ID (ms)**	**Chem ID (ms)**	**Phy ID (ms)**	**Chem ID (ms)**	**Phy ID (ms)**	**Chem ID (ms)**	**Phy ID (ms)**	**Chem ID (ms)**
778	5.58	3.1	3.52	1.79	3.4	1.57	3.1	1.33
788	4.92	2.8	3.26	1.64	3.16	1.48	2.88	1.25
798	4.76	2.68	2.82	1.57	2.84	1.37	2.66	1.16
808	4.5	2.5	2.66	1.50	2.6	1.34	2.5	1.14
818	4.22	2.44	2.54	1.38	2.48	1.27	2.34	1.08
828	4.06	2.34	2.42	1.36	2.34	1.19	2.18	1.06
838	4.02	2.06	2.32	1.29	2.26	1.14	2.12	1.03
848	3.96	2	2.16	1.24	2.12	1.10	2	1.01

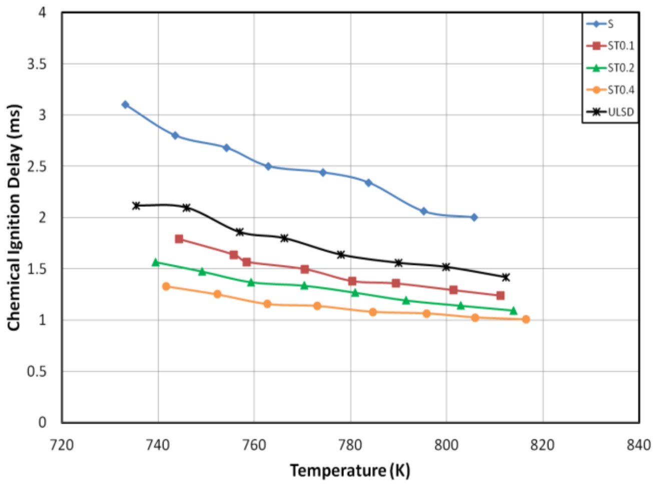


Figure 12 – Chemical ignition delay at mean temperature for different fuels

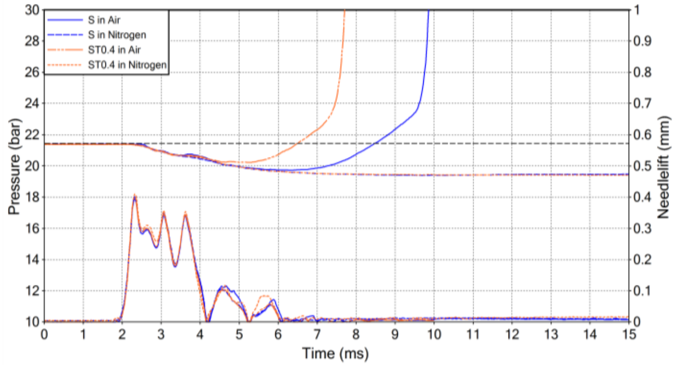


Figure 13 – Pressure and needlelift traces in air and nitrogen charge at temperature 818 K

Figure 13 shows the pressure and N.L traces for (S) and (ST0.4) injection into air and into nitrogen at a charge temperature of 818K. It is observed that the POI is more advanced in (ST0.4) than (S). This implies that the additive accelerates the initiation reactions in the early stage of the autoignition process [10,41]. In other words, the cetane improver enhances the radical pool formation in the early stage and provides an efficient mechanism of exothermic reactions [10,41]. Thus, the exothermic reactions start much earlier in the fuel with additives.

ARRHENIUS PLOT AND APPARENT ACTIVATION ENERGY

The Arrhenius plot is developed for the chemical ID versus the reciprocal of the absolute integrated mean temperature (in Kelvin) during the chemical ID period. The apparent activation energies can be determined from Eqn. 3 .

$$Ln\left(\frac{1}{ID}\right) = LnA - \frac{1000E_a}{R_u T} \tag{3}$$

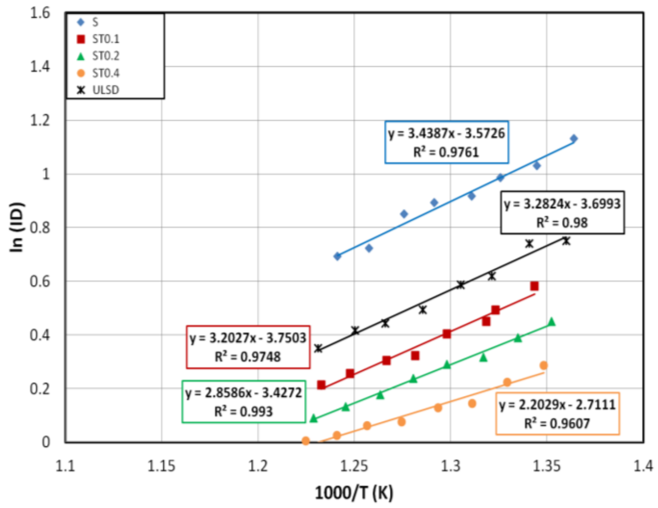


Figure 14 – Arrhenius plots for chemical ignition delay versus the mean temperature for (S) and STs)

Table 4 – Apparent activation energy for (S) and STs)

Fuel	Apparent activation energy Ea (kJ/mole)
(S)	28.574
(ST0.1)	26.613
(ST0.2)	23.753
(ST0.4)	18.305
ULSD	27.310

It should be noted that the activation energies calculated from Figure 14 do not represent elementary chemical reactions but rather a large number of known, unknown, simple and complex chemical reactions that occur during the autoignition process [42]. The apparent activation energies, Ea, of different fuels calculated from Figure 14 are given in Table 4.

Table 4 shows that (ST0.4), which has the shortest chemical ID, has the highest CN and lowest activation energy of 18.305 kJ/mole. Meanwhile, (S), which has the longest ID, has the lowest CN and the highest activation energy of 28.574 kJ/mole. ULSD has an activation energy of 27.31 kJ/mole, which is lower than (S) but higher than the others. It should be noted that exothermic reactions of low activation energy fuels take place earlier than high activation energy fuels.

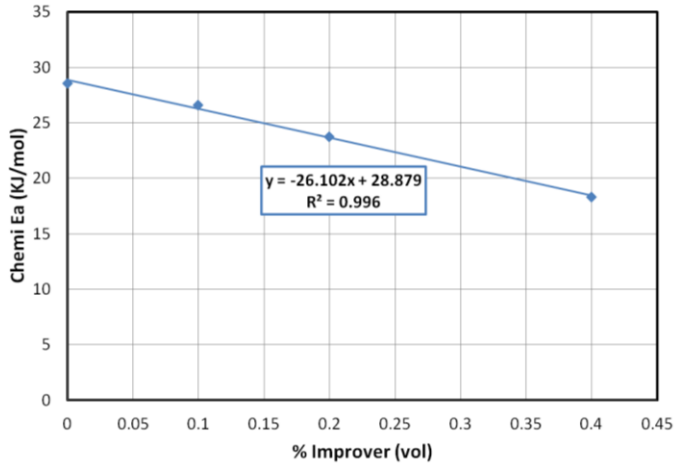


Figure 15 – Correlation between activation energy based on the chemical delay and concentration of cetane improver

Figure 15 shows the correlation between the apparent activation energy and the percentage of the cetane improver. The figure shows the activation energy based on the chemical ID decreases linearly with the increase in the percentage of the added cetane improver used in this investigation.

CONCLUSIONS

The following conclusions are based on an experimental investigation on the effect of treating the low cetane Sasol IPK fuel with percentages of 2-EHN (2-ethylhexyl nitrate cetane improver) ranging from 0.1% to 0.4%. The experiments were conducted in the constant volume vessel of the Ignition Quality Tester (IQT) at a constant pressure of 2.14 MPa and temperatures varying from 778 to 848 K.

1. DCN (Derived Cetane Number) of Sasol IPK increased from 31.1 to 41.5 (a gain of 10.4 units) by adding 0.4% of Lubrizol 8090 cetane improver to the fuel.
2. The highest gain of 6.8 in DCN was achieved by adding the first 0.1% of the additive. The gain decreased gradually by adding higher percentages of the additive.
3. A detailed analysis of the RHR during the autoignition process showed the impact of the additive on accelerating the early initiation reactions, leading to the LT regimes, as well as exothermic

reactions, leading to the high temperature combustion.

4. Treating the fuel with the additive reduced the ID at different charge temperatures. However, the LT regimes observed in the autoignition of the base fuel were present with the treated fuel.
5. For the original and treated fuel, the higher the charge temperature, the less effective was the additive in reducing the ID.
6. The apparent activation based on the chemical ID decreased linearly with the increase in the percentage of the added cetane improver.

NOMENCLATURE

A	Pre-exponential factor
AET	Advanced Engine Technology
ARHR	Apparent Rate of Heat Release
CFR	Cooperative Fuel Research
CI	Compression Ignition
CN	Cetane Number
DAQ	Data Acquisition
DCN	Derived Cetane Number
Ea	Apparent Activation Energy
EGR	Exhaust Gas Recirculation
HMN	Hepta-methyl-nonane
ID	Ignition Delay
IQT	Ignition Quality Tester
LT	Low Temperature
NI	National Instrument
NL	Needlelift
NTC	Negative Temperature Coefficient
POI	Point of Inflection
RANS	Reynold Average Navier-Storkes
RHR	Same as ARHR
$\mathbf{R_u}$	Universal Gas Constant
SOI	Start of Injection
S	Sasol IPK
ST0.1	Sasol IPK treated with 0.1% cetane improver
ST0.2	Sasol IPK treated with 0.2% cetane improver
ST0.4	Sasol IPK treated with 0.4% cetane improver
STs	Cetane improver treated fuels
SwRI	Southwest Research institute
TDC	Top Dead Center
ULSD	Ultra-Low-Sulfur-Diesel
WSU	Wayne State University

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APPENDIX A

Table A.1

Standard Deviation of ignition delay and test temperature for different fuels

	S		ST0.1		ST0.2		ST0.4	
Test T (K)	**Std Dev ID**	**Std Dev Temp**	**Std Dev ID**	**Std Dev Temp**	**Std Dev ID**	**Std Dev Temp**	**Std Dev ID**	**Std Dev Temp**
778	0.183	0.2	0.235	0.2	0.189	0.2	0.125	0.2
788	0.156	0.2	0.207	0.2	0.244	0.2	0.134	0.2
798	0.179	0.2	0.101	0.233	0.148	0.2	0.107	0.233
808	0.175	0.2	0.152	0.233	0.136	0.233	0.098	0.233
818	0.156	0.266	0.131	0.233	0.139	0.2	0.111	0.233
828	0.15	0.2	0.099	0.2	0.102	0.233	0.073	0.2
838	0.105	0.233	0.09	0.2	0.116	0.233	0.077	0.2
848	0.08	0.233	0.105	0.2	0.072	0.2	0.082	0.2

Table A.2

Repeatability and Reproducibility Values for Information

ID (ms)	Repeatability (r)	Reproducibility (r)
3.1	0.030	0.158
3.6	0.055	0.198
4.2	0.085	0.246
4.8	0.115	0.293
6.0	0.175	0.388
6.5	0.200	0.428
DCN	Repeatability (r)	Reproducibility (r)
33	0.67	1.96
40	0.77	2.23
45	0.83	2.43
50	0.90	2.62
55	0.96	2.81
60	1.03	3.00
64	1.08	3.16

APPENDIX B

Properties of 2- ethylhexyl nitrate (2EHN) additive

IUPAC name	2- ethylhexyl nitrate (2EHN)
Molecular formula	$C_8H_{17}NO_3$
Molecular weight	175.23
Flash point	>70℃(closed-cup)
Freezing point	<-45℃
Boiling point	>100℃(decomposes)
Vapor pressure	27Pa@20℃
Vapor pressure	40-53Pa@40℃
Vapor pressure	1.33Pa@82℃
Density	0.96g/ml@20℃
Kinematic viscosity	1.8cSt@20℃
Solubility in water	12.6g/ml@20℃
Heat of vaporization	368kJ/kg
Coefficient of thermal expansion (between 10 ℃and 20 ℃at atmospheric pressure)	1.010
Auto/Self ignition temperature	130℃(decomposes)
Decomposition temperature	>100℃

Fuel Properties

Fuel	ASTM	ULSD	Sasol
Cetane Number	D613	42.3	25.4
Derived Cetane Number	D6890	42.1	31.1
Flash point (℃) min	D93	69	42
Density (@15 ℃) kg/m3	ASTM 85H	842	755
Viscosity (cSt, 40 ℃)	D445	2.438	1.125
Heating Value (MJ/kg)	D4809	41.2	44.0
Aromatic content (%Mass)	D2425	27.8	0.2