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Effect of Initial and Operating Conditions on Soot Emissions from an HCCI Engine

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1. Summary

Homogeneous Charge Compression Ignition (HCCI) combustion is generally characterized by near-zero soot and NO_x emissions. For this reason, this combustion strategy is being considered for use in advanced technology engines in order to meet increasingly stringent emissions regulations. However, soot can be produced in an HCCI engine due to in-cylinder composition (air-fuel ratio, exhaust gas recirculation rate) or non-uniformities in temperature. In this study, soot emissions from an HCCI engine were measured by laser-induced incandescence (LII) over a range of initial and operating conditions using an ultra-low sulphur diesel fuel.

A variable compression ratio Cooperative Fuels Research (CFR) engine connected to an eddy-current dynamometer was used for these experiments. The engine was equipped with an air-blast atomizer and vaporizer in the intake manifold to prepare the fuels prior to entering the combustion chamber. A cooled exhaust gas recirculation (EGR) loop and simulated turbocharging were provided as means to dilute the combustion process. Soot emissions from the engine were measured with a range of fuel vaporizer temperatures, in-cylinder compositions (air-fuel ratio, exhaust gas recirculation rates) and engine speeds.

It was found that soot emissions increased rapidly when the vaporizer temperature was reduced below 200°C using a commercial ULSD fuel. Soot emissions also increased at lower engine speeds. Soot emissions were found to increase as the air-fuel ratio was decreased toward the knocking limit and the EGR rate was reduced. Knocking led to significantly higher soot emissions. This is a significant challenge because the highest fuel conversion efficiency occurs near the knocking limit.

2. Introduction

Unlike conventional diesel combustion engines, homogeneous charge compression ignition (HCCI) combustion offers the potential of near zero NO_x and soot emissions.¹⁻⁴ HCCI combustion can be achieved either by premixing fuel in the intake or by direct injection of the fuel early in the compression stroke. For premixed HCCI combustion, n-heptane has been used widely as it can be atomized in the intake system with relatively low injection pressure.⁵ Regular diesel fuels can be injected directly into the cylinder early in the compression stroke by means of a common rail diesel fuel injection system.⁶ However, the option of diesel-fueled premixed HCCI combustion has not yet been examined extensively due to the inherent technical difficulty of atomizing/vaporizing diesel fuel inside the intake port at low port fuel injection pressures. In doing so, there is a high likelihood of in-homogeneity and incomplete fuel vaporization that could cause soot emissions even in fully premixed HCCI combustion. Thus, while HCCI is known for soot-free combustion, under some operating conditions soot formation can occur and it is unlikely to be oxidized at characteristically low HCCI combustion temperatures.

The objective of this study is to explore the limits under which soot is produced in fully-premixed HCCI combustion and to identify the effect of operating parameters on soot emissions. Also, it is aimed at finding any possible interaction between soot, other emissions and engine operating parameters.

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3. Experimental setup

The Cooperative Fuels Research (CFR) engine used for this study is a single-cylinder, four-stroke, variable compression ratio engine with bore \times stroke of 82.55 \times 114.3 mm. The engine setup was modified from the standard CFR configuration by the addition of an air- assist port fuel injection system and hardware to control critical engine parameters such as intake temperature, air/fuel ratio, intake and exhaust pressures, and exhaust gas recirculation. An in-house fuel vaporizer was fitted to the outlet of the fuel injector to vaporize the lighter diesel fuel components, which permitted HCCI combustion with near-zero soot emissions. Figure 1 shows details of the fuel injector/vaporizer. The fuel vaporizer is capable of delivering the fuel spray at any point within a wide temperature band. By adjusting the fuel vaporizer temperature (T_{vap}) it is possible to determine the fraction of vaporized fuel to total fuel per injection. Operating at low T_{vap} causes incomplete vaporization, and hence, the potential for soot particles in the exhaust stream. Operation at high T_{vap} causes fuel fouling on the heater surfaces inside the vaporizer. Hence, based on fuel properties (mostly volatility), a minimum critical temperature may be determined for each fuel to avoid soot emissions while keeping the temperature below fuel fouling limits. The low and high temperature limits of the fuel vaporizer are the subject of a separate study.

All experiments were performed under steady state conditions. An AVL 415 Variable Sampling Smoke Meter and an Artium Technology LII 200 were used to measure soot emissions. The cylinder pressure data was acquired with 0.2 CAD resolution for 300 consecutive engine cycles. Combustion parameters and resultant statistics were calculated for all 300 collected cycles.

4. Results and discussion

LII measurement limits

LII was used to study soot emissions at extremely low concentrations which were not detectable with the low sensitivity AVL smoke meter. Single shot LII measurements were made at a 20 Hz rate over a sample period of 180 s. For comparison, three sample cases of operating conditions 6, 7, and 10 were selected from the experimental data shown in Figure 3 which represent increasing soot emission rates, with the relative highest being the only one detectable with the AVL smoke meter. Figure 2 compares the soot measurements in the three cases using the LII instrument with the upper plots showing soot mass concentration (SMC) as a function of time and the lower plots represent the same information as histograms with statistics. From Figure 2-a to Figure 2-c, SMC increases by an order of magnitude. In Figure 2-a, the measurements are scattered without a particular pattern and the statistical analysis indicated a standard deviation greater than mean. For the intermediary case 7, in Figure 2-b, the SMC was more than 0.02 mg/m^3 and LII measurement appear less scattered though the standard deviation was about 50% of the mean.

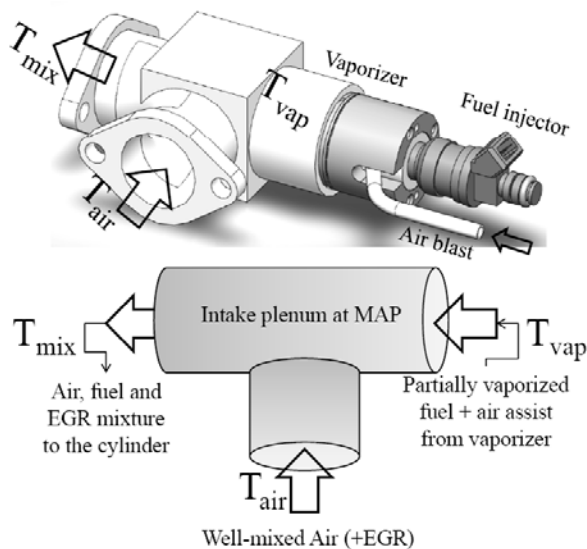


Figure 1: Schematic of enhanced fuel injector/vaporizer.

For the highest soot emissions case 10, shown in Figure 2-c, a normal distribution of values for SMC with low standard deviations is observed. It is concluded that the LII 200 instrument cannot accurately report soot emissions below 0.02 mg/m^3 .

Effect of fuel vaporizer temperature

The temperature of the fuel vaporizer can be controlled to achieve increasing levels of fuel vaporization. For each fuel, the degree of vaporization was monitored using the AVL smoke meter while increasing the vaporizer temperature. During the tests all initial conditions were kept constant while T_{air} was adjusted relative to T_{vap} such that T_{mix} remained constant. Figure 4 exhibits the vaporizer temperature effect on soot formation in HCCI combustion for a fuel at $T_{mix} = 61^\circ\text{C}$.

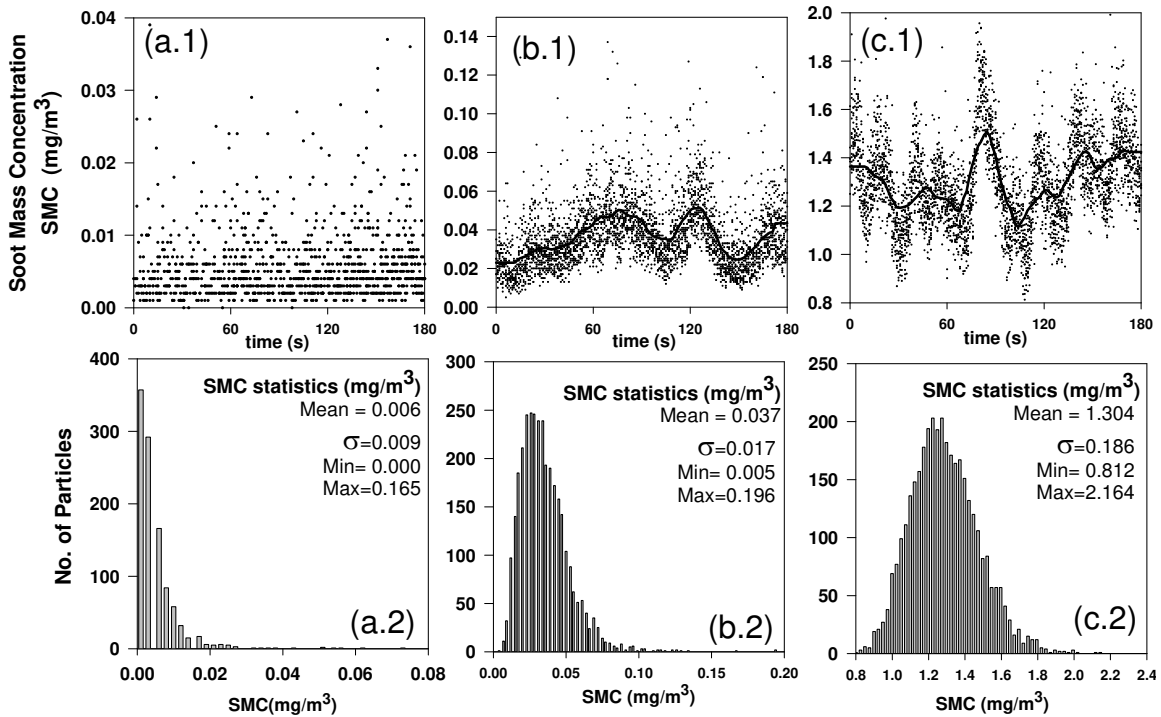


Figure 2: soot mass concentration (SMC) measured over the period of 180 s, Statistical analyses for three cases of points 6, 7, and 10 of Figure 4. ULSD, N=900 rpm, EGR=0%, AFR=51.0, CR=11.0.

Data obtained by both AVL smoke meter and LII are shown for comparison. It is observed that when the vaporizer temperature increases above a certain threshold value, the soot concentration of the engine exhaust stabilizes at a low constant level which remains insensitive to vaporizer temperature over a broad temperature range. However, below the threshold, soot concentration in the exhaust stream increases with decreasing vaporizer temperature. The transition point is called the fuel vaporizer critical temperature (T_{cr}) in this paper.

The influence of EGR on T_{cr} is summarized in Figure 5 that includes the complete data range and a magnified sub-section. Increasing EGR fraction from 10% to 60% reduced T_{cr} . As an example, if the soot emissions limit is assumed as 0.2 mg/m^3 , T_{cr} was reduced from 199.3°C to 197.7°C , when the EGR fraction was increased from 20% to 40%. At very high EGR fractions, no soot formation occurred at very low T_{vap} due to the low combustion temperature. However, it should be noted that HC and CO emissions were extremely high when excessive EGR was used. The influence of EGR on soot emissions is discussed in greater detail below.

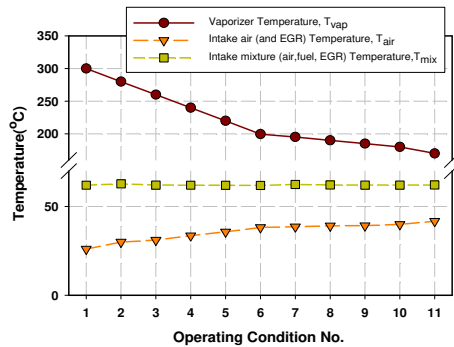


Figure 3: The operating temperatures for the vaporizer temperature sweep, ULSD, N=900 rpm, EGR=0%, AFR=51.0, CR=11.0.

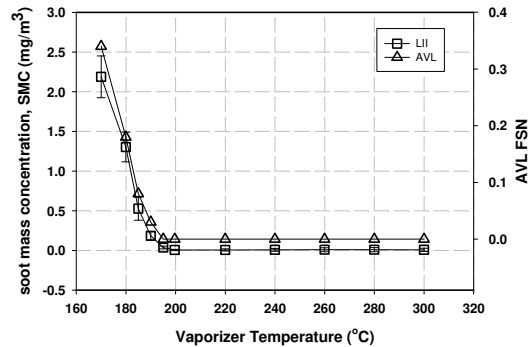


Figure 4: Determining the minimum vaporizer temperature based on soot emissions data. ULSD, N=900 rpm, EGR=0%, AFR=51.0, CR=11.0. Note that the Y-axis scale for the AVL FSN is slightly shifted.

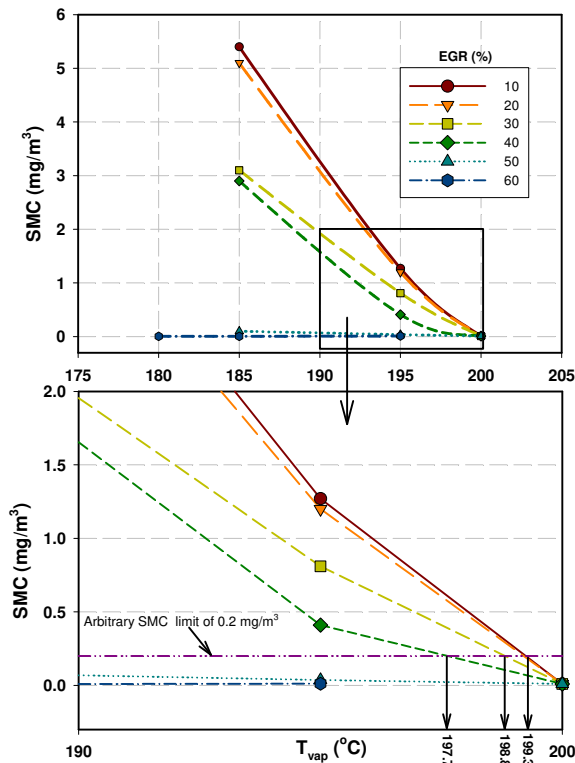


Figure 5: Effect of EGR on fuel vaporizer critical temperature (T_{cr}) for soot-free combustion.

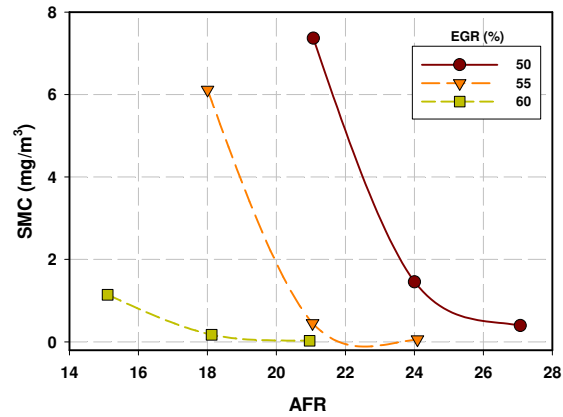


Figure 6 : Effect of AFR and EGR on soot mass concentration. ULSD, $N=900$ rpm, $CR=10.0$, $T_{vap}=195$ °C, $MAP=200$ kPa, $T_{mix}=70$ °C.

Clearly, the phenomena observed in Figure 4 were caused by the incomplete vaporization of fuel. When the vaporizer temperature decreases beyond T_{cr} , more fuel droplets form and enter the cylinder, creating fuel-rich pockets. These in turn enhance the formation the soot. Above T_{cr} , all fuel is vaporized in time to be burned during the main combustion stage and a constant low level of soot emission is observed.

Combined effect of EGR and AFR on soot emissions

Figure 6 shows the combined effect of AFR and EGR on soot emissions. The vaporizer temperature was set at 195°C to have detectable levels of soot while examining the AFR-EGR operating region. At any constant AFR, soot concentration decreased with increasing EGR. This is caused by several factors. Firstly, the addition of EGR reduces the concentrations of fuel (at any constant AFR level) which in turn reduces soot precursors, which results in a lower soot formation rate. Secondly, the higher specific heat of EGR (triatomic molecules of H_2O and CO_2 replace diatomic N_2 molecules) reduces compression and peak combustion temperatures which result in reduced soot formation and oxidation rates. In low to medium EGR ranges, the soot oxidation rate is reduced more than the soot formation rate, and hence increased soot emissions are observed in conventional diesel combustion. However, at high EGR rates (typical of HCCI combustion conditions), the soot formation rate becomes so low that the effect of the reduced soot oxidation rate becomes insignificant.⁷ Lastly, some components of EGR, such as CO_2 , H_2O and CO , may participate in chemical reactions. For example in a numerical study of a counter flow diffusion flame, Liu et al.⁸ showed that CO_2 participates in chemical reactions by suppressing chemical soot formation through reducing the concentration of acetylene and flame temperature and the conversion of CO_2 by hydrogen atom to hydroxyl, in turn prompting oxidation of soot precursors in the soot formation region. Further, it was shown by Guo et al.⁹ that the chemical effects of CO_2 addition suppresses soot inception and surface growth rate, but has negligible effect on the soot oxidation process.

Although some researchers argue that the addition of EGR may slow the oxidation of soot particles and thus increase soot emission, apparently this is not the case in HCCI combustion. This seems to be the key difference between soot formation in conventional diesel combustion and premixed HCCI combustion. In conventional diesel combustion, any attempt to decrease NOx formation by increasing EGR, decreases soot oxidation during the expansion stroke resulting in an increase in soot emissions. Huestis et al.⁷ reported that by increasing EGR from 21% intake O_2 concentration to 12% intake O_2 concentration, soot was increased, but further EGR increase to 8% intake O_2 concentration reduced soot. Below 8% intake O_2 concentration, soot was not detectable with the in-cylinder optical soot measurement method. The same trend was reported by Idicheria et al.,¹⁰ and Tao et al.¹¹

At any constant EGR rate, soot concentration increases with decreasing AFR. This is caused by three factors. Firstly, fuel vapor pressure is increased with decreasing AFR, leading to a lower vaporization rate.

Secondly, decreasing AFR creates higher in-cylinder temperature enhancing soot formation. Lastly, lower AFR equates to higher carbon content of the mixture, which promotes soot formation reactions.

Effect of engine speed on soot emissions

Figure 7 illustrates the effect of engine speed on soot emissions. Speed sweeps were performed twice. First, T_{mix} was kept constant and speed was increased while CA50 was not controlled. Then, while the speed was increased, CA50 was kept constant by increasing T_{mix} . As indicated in Figure 7, the results are largely the same for the two methods with soot mass concentration decreasing with increasing engine speed.

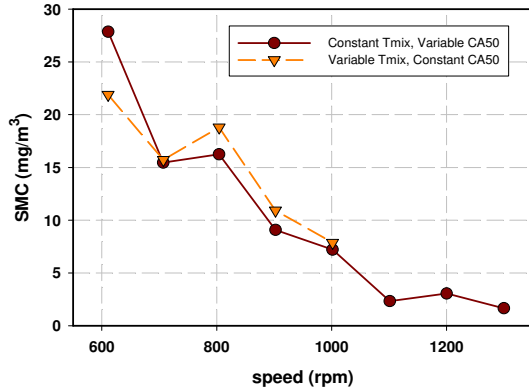


Figure 7: Effect of speed on soot mass concentration, ULSD, CR=10.0, T_{vap} =195°C, EGR=42%, AFR=26.

The mixing process between fuel-rich zones and lean zones is intensified with increasing engine speed. This may be the primary reason that soot concentration decreases with increasing engine speed. In addition, increasing engine speed also decreases the residence time of the mixture inside the cylinder, slightly decreases the peak combustion temperature and hence, it reduces both soot formation rate and soot formation. It is interesting to note that soot concentration decreases with increasing engine speed even when CA50 is constant by adjusting T_{mix} . This suggests that the effect of engine speed on soot emissions is stronger than both combustion timing and mixture temperature under the examined conditions.

Table 1: constant speed-load conditions.

| | Speed =900 rpm | Speed=1250 rpm | Speed =1600 rpm | |
|--------------|----------------|----------------|-----------------|--------------|
| IMEP =6 bar | Mode 1 | Mode 4 | Mode 7 | MAP = 2 bar |
| IMEP = 4 bar | Mode 2 | Mode 5 | Mode 8 | MAP =1.5 bar |
| IMEP = 2 bar | Mode 3 | Mode 6 | Mode 9 | MAP =1.0 bar |

Soot emissions at constant speed-load conditions

A set of constant speed-load conditions were examined using four various diesel fuels. Table 1 illustrates the experimental conditions for constant speed-load conditions.

Figure 8 shows the effect of operating conditions on soot emissions. Figure 8-b is a magnification of Figure 8-a. Most of experimental results as indicated in Figure 8-b are below the LII 200 SMC measurement confidence level of 0.02 mg/m³ as discussed under Figure 3. However, a general trend of decreased soot as load is decreased can be observed. Note that according to Table 1, load is decreased at constant speed from modes 1 to 3, modes 4 to 6, and modes 7 to 9.

The same trend is observed for SMC in Figure 8-b. It is difficult to obtain a trend for effect of fuel chemistry (in this case the effect of processing severity of oil sands diesel fuels) on soot emissions. However the highest cetane number fuel (which was also the most volatile) produced the lowest soot emissions.

Soot-NOx relationship

The NOx-soot trade-off has been studied mostly for diffusion flames and conventional diesel combustion systems due to the inherent difficulty of achieving simultaneous reduction of NOx and soot emissions.¹² Typically both NOx and soot emissions are extremely low in HCCI combustion. Figure 9 shows the relation between NOx and soot while the vaporizer temperature sweep was performed. With decreasing vaporizer temperature, both NOx and soot increased considerably. The increase in soot emissions has been explained above. Numerical simulations by Guo et al^{13, 14} in ethylene/air diffusion flames have indicated that while NOx formation does not have a significant effect on soot, soot formation affects NOx emissions through the radiation induced thermal effect and the reaction induced chemical effect.

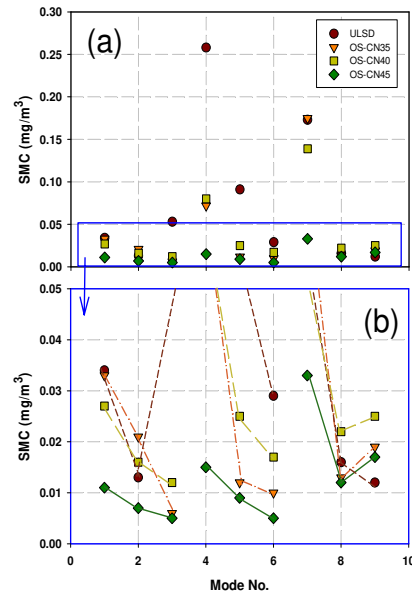


Figure 8: SMC examined in the constant speed-load conditions of Table 1.

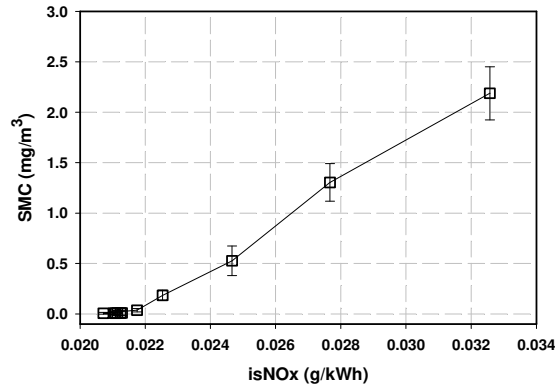


Figure 9 : NOx-soot relationship observed when varying the vaporizer temperature, ULSD, N=900 rpm, EGR=0%, AFR=51.0, CR=11.0.

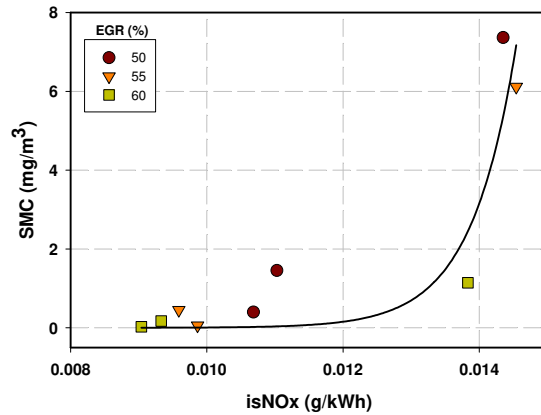


Figure 10: NOx-soot relationship while examining combined effects of AFR and EGR, ULSD, N=900 rpm, CR=10.0, $T_{vap}=195\text{ }^{\circ}\text{C}$, MAP=200 kPa, $T_{mix}=70\text{ }^{\circ}\text{C}$.

While the vaporizer temperature was decreased, the increased NOx emissions may have been driven by NO formation due to the prompt route enhanced by the existence of the fuel-rich spots. When the vaporizer temperature was higher than the critical value, both soot and NOx emissions did not significantly change with varying vaporizer temperature.

In the AFR-EGR operating region, both NOx and soot increased with decreasing AFR and/or EGR (Figure 10). The reason for the increase in soot emissions has been explained before. NOx formation is highly sensitive to combustion temperature. The substantial increase in soot and NOx emissions on the right hand side of Figure 10 is due to the increase in flame temperature when AFR is decreased.

Increases in engine speed resulted in decreases in both NOx and soot emissions, as indicated in Figure 11. The effect of engine speed on HCCI combustion characteristics has been discussed (Hosseini et al ¹⁵) as decreased LTHR activity and consequently retarded combustion timing. The effect of engine speed on NOx is not clear, as under certain conditions NOx emissions increased, decreased, or remained constant. Figure 11 suggests that NOx emissions monotonically decreased with a decrease in soot emissions. Both soot and NOx emissions decreased with increasing engine speed. As mentioned, we have not found a consistent correlation of NOx emissions with engine speed. However, in this case, as soot was intentionally introduced in the experiment (by operating the vaporizer below the critical temperature limit), the trends observed with NOx emissions appeared coupled to the soot emissions trends and tied to the existence of fuel rich mixtures during engine conditions which favored soot formation.

A transient experiment was performed where the compression ratio was continuously increased from CR=11.0 to CR=13.0 over a 40 second period at a constant engine speed of 900 rpm and while all other initial conditions remained constant. Because of increasing compression ratio, combustion timing (CA_{50}) was advanced from $-4\text{ }^{\circ}\text{CA}_{aTDC}$ to $-18\text{ }^{\circ}\text{CA}_{aTDC}$. Due to advancing the combustion timing from the optimum value ($0\text{ }^{\circ}\text{CA}_{aTDC}$) to earlier combustion timing, IMEP was decreased from 4.8 bar to 3.6 bar.

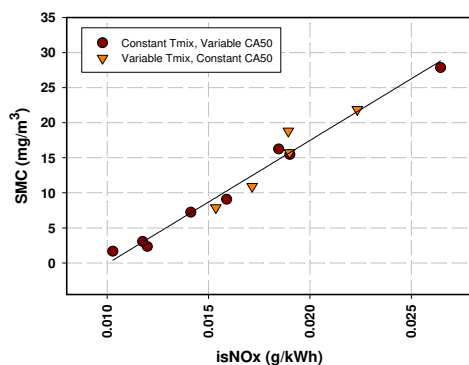


Figure 11: NOx-soot relationship for a range of engine speeds, ULSD, CR=10.0, $T_{vap}=195\text{ }^{\circ}\text{C}$, EGR=42%, AFR=26

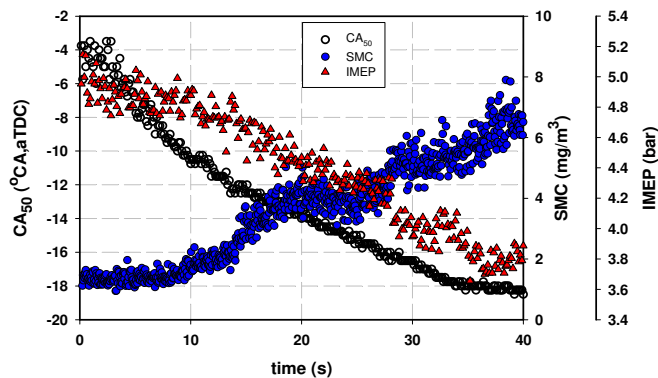


Figure 12: Effect of compression ratio and combustion timing on soot emissions

Simultaneously, SMC was increased from almost zero to more than 6 mg/m^3 which is a substantial soot emission for HCCI combustion. Meanwhile NO_x emissions were increased, but due to the delayed sampling and analysis response were not correlated with other data in Figure 12.

5. Conclusions

- Although HCCI combustion is known for near zero soot emissions, under certain conditions with regular diesel fuels, it is possible to produce significant soot concentrations in the exhaust. This is an important result of this study as most of diesel HCCI combustion experiments have been performed with volatile hydrocarbons (such as n-heptane) and not real diesel fuels. Soot emissions are often not being measured or reported.
- LII measurements of soot concentration were sampled from the exhaust stream of an HCCI combustion engine operating with a series of diesel fuels. Measurement was reasonably repeatable for $\text{SMC} > 0.02 \text{ mg/m}^3$.
- Decreasing AFR toward the rich limit and decreasing EGR both increased soot emissions. This is a particularly important observation as the most efficient HCCI combustion happens near the knocking limit. Knocking was strongly coupled with soot emissions.
- Soot emissions were higher at lower engine speeds. The engine speed effect was stronger than that of combustion timing and intake mixture temperature.
- The conventional diesel combustion NO_x-soot trade-off was not observed in HCCI combustion. Instead, NO_x and soot emissions appeared to be coupled. Specifically, conditions where soot was formed also led to increased NO_x formation.
- Generally, HCCI combustion happens in a region in which the peak combustion temperature is below the NO_x formation threshold temperature and above the soot formation threshold temperature. Further decreases in peak combustion temperature (for example by increasing EGR and/or AFR) may reduce soot emissions further.

Nomenclature

| | |
|------------------------|---|
| AFR | Air fuel ratio |
| CR | Compression ratio |
| LII | Laser Induced Incandescence |
| LTHR | Low temperature heat release |
| MAP | Manifold absolute pressure |
| SMC | Soot mass concentration (mg/m^3) |
| T_{air} | Intake air (and EGR) temperature |
| T_{mix} | Intake mixture (air, fuel, and EGR) temperature |
| T_{vap} | Fuel vaporizer temperature |
| ULSD | Ultra low sulphur diesel |

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