

Analysis of the Correlation Between Engine-Out Particulates and Local Φ in the Lift-Off Region of a Heavy Duty Diesel Engine Using Raman Spectroscopy

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ABSTRACT

The local equivalence ratio, Φ , was measured in fuel jets using laser-induced spontaneous Raman scattering in an optical heavy duty diesel engine. The measurements were performed at 1200 rpm and quarter load (6 bar IMEP).

The objective was to study factors influencing soot formation, such as gas entrainment and lift-off position, and to find correlations with engine-out particulate matter (PM) levels. The effects of nozzle hole size, injection pressure, inlet oxygen concentration, and ambient density at TDC were studied. The position of the lift-off region was determined from OH chemiluminescence images of the flame. The liquid penetration length was measured with Mie scattering to ensure that the Raman measurement was performed in the gaseous part of the spray.

The local Φ value was successfully measured inside a fuel jet. A surprisingly low correlation coefficient between engine-out PM and the local Φ in the reaction zone were observed. This indicates that the soot forming rate is not the dominant factor behind the trends in engine-out PM. High correlation coefficients between PM and; portion of heat release after end of injection (EOI), engine out UHC and engine out CO all suggests that the soot oxidation process may be a more important factor.

INTRODUCTION

Compared with Otto engines, Diesel engines benefit from higher efficiency but also produce more emission. Increasing oil prices stress the importance of efficiency, while emission regulations continue to tighten. A deeper understanding of the combustion process may make it easier to reach stringent emission targets with maintained efficiency.

Heavy duty diesel engines tend to be operated at high loads where the long injection durations produce a combustion process that is largely spray-driven. A useful picture for understanding emission formation in these engines is that of a lifted flame on a stationary jet. This is because the diesel spray can be considered to behave as a quasi-stationary jet during the major part of combustion. It is well known that engine-out particulate matter (PM) levels from these engines can be controlled using elevated injection pressures, decreased injector orifice size, increased ambient density and cooled exhaust gas recirculation (EGR). With the latter method it is the combination of dilution and cooling that improves the Nitrogen oxides (NO_x)-PM trade-off. This investigation analyses the effects of these engine parameters on the quasi stationary jet characteristics.

Engine-out PM emissions can be seen as the result of two competing processes: soot forming and soot oxidation. The amount of soot produced depends on the soot forming rate and the residence time. The soot

forming rate mainly depends on two variables: the combustion temperature and the equivalence ratio, Φ . Soot is mainly formed at temperatures above 1700 K in zones where $\Phi > 2$ [1]. Entrainment of hot air upstream of the lifted diffusion flame is therefore important for the soot forming in the jet. This is because the amount of air entrained determines the equivalence ratio and the temperature in the interior of the jet. After the flame lift-off length entrainment of ambient air is impeded by the diffusion flame. The local Φ in the lift-off region therefore gives information about the soot forming process [2,3,4,5,6].

Due to the continuous entrainment of ambient gas into the fuel jet, Φ varies with the distance from the injector orifice. It can be estimated by EQ (1), developed by Siebers and coworkers [7,8]. The expression was derived applying conservation of mass and momentum principles to an idealized model of a jet. The model assumes a constant spreading angle, α radially uniform velocity and fuel concentration profiles, and no velocity slip between the injected fuel and the ambient gas. According to this simplified analysis, Φ varies as

$$\Phi(x) = \frac{2(A/F)_{st}}{\sqrt{1 + 16\left(\frac{x}{x^+}\right)^2 - 1}}, \quad (1)$$

where $(A/F)_{st}$ is the stoichiometric air-fuel ratio, which is approximately 15 for diesel fuel. The denominator contains the axial location, x , and the characteristic length, x^+ , that is used to simplify the expression.

$$x^+ = \sqrt{\frac{\rho_f}{\rho_a}} \frac{\sqrt{C_a} d}{\tan(\alpha/2)}, \quad (2)$$

where ρ_f and ρ_a are the fuel and ambient gas densities, respectively. The area contraction coefficient C_a and the hole diameter d are related to the nozzle geometry. The jet spreading angle, α , depends only on the fuel and ambient gas densities. In the current investigation the local Φ was measured in the centre of the jet using Raman spectroscopy. It should be noted that these values cannot be directly compared with the Φ -values from EQ (1), which are averages over the jet cross section, but they should correspond to each other qualitatively.

Φ -measurements have been made in diesel engines before [2,9,10,11,12,13]. The current measurements included variations in EGR rate, injection pressure, nozzle orifice diameter, and ambient gas density. The aim was to find the most important factors affecting the local Φ in the jet and thereby cast light on the origin of observed engine-out PM trends. The equations above were used in the analysis for relating the measured results to the current understanding of air entrainment in sprays.

Besides PM, other emissions were also studied. NO_x , unburned hydro carbons (UHC) and carbon monoxide (CO) were measured. NO_x forming is less complicated than soot forming. In diesel engines it is dominated by the thermal, so-called Zeldovich mechanism. According to this NO_x is formed most rapidly at high temperatures at slightly lean conditions. The reactions are relatively slow and therefore the mixture that burns early during the cycle is the dominating source of NO_x . The reactions usually freeze when the temperature drops during expansion, leading to engine-out emissions far above the equilibrium concentration [14].

UHC and CO are less of an issue for heavy duty diesel engines but are still interesting to investigate. The UHC-sources can be divided into four major sources; rich zones, over lean zones, cold zones near walls, and fuel from the sac volume of the injector. Engine-out CO mainly becomes a problem if the final combustion stages have not been completed before the bulk temperature drops below approximately 1500 K in the expansion stroke. The oxidation of CO to carbon dioxide (CO_2) can then not be completed [14,15].

METHOD

The setup and evaluation of the measurements presented here was done using Design of Experiments (DoE). A central composite design, based on a two-level full factorial design with superimposed axial and center points was chosen for the experiments. A more detailed description of these designs and their properties can be found in [16]. The experimental variables were the injection pressure, the ambient density at top dead centre (TDC), the inlet oxygen concentration and the inlet temperature. During the initial factor screening the inlet temperature was swept from 85 °C to 115 °C, corresponding to a TDC temperature range of over 70 °C for a motored cycle. The inlet temperature was decided to be excluded from the experiment because it had almost no impact on the emissions

The settings of the variables are given in Table 1 and graphically in Figure 1. The levels were chosen to give significant responses in engine-out emissions, mainly in PM. The test matrix consisted of 15 operating points per injector as seen in Table 2. This relatively small data set may seem too sparse for the analysis, but using DoE the experiment is mathematically designed to provide certain information from the least number of measurements possible. It should be noted that with DoE *all* the observations are used to estimate *each* of the factor effects. In the current experiment this means that each factor effect is determined using a fivefold replicate experiment (there are five measurements at each factor level). To obtain equal precision, a traditional experiment would have required fifteen measurements for each factor, i.e. 45 measurements in total.

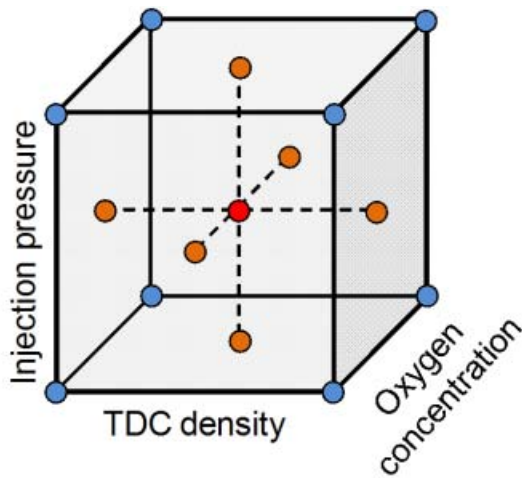


Figure 1 Graphical representation of the experimental factors and their levels. Blue points are the corner points of the central composite design. The red point is the center point and orange points are axial points.

Table 1 Engine control parameters.

	Low (-)	Base (0)	High (+)
Rail pressure [bar]	1500	2000	2500
Inlet O ₂ conc. [%]	12	14	16
p at TDC [kg/m ³]	24	27	30

In traditional experiments, one factor is changed at a time. The effect of a single factor is thus estimated at selected and fixed conditions of the other factors. For such an estimate to have general relevance one must assume that the effect is the same at different settings of the remaining factors, i.e. that the factors affect the response additively. If they *do* act additively, DoE estimates the effect with more precision. If they *do not* act additively, DoE (unlike traditional experiments) can detect and estimate interactions that measure this non-additivity [16].

Table 2 Measurement matrix in coded values.

Case	Inlet O ₂ concentration	p at TDC	Injection pressure
1	+	+	+
2	-	+	+
3	+	-	+
4	-	-	+
5	+	+	-
6	-	+	-
7	+	-	-
8	-	-	-
9	+	0	0
10	-	0	0
11	0	+	0
12	0	-	0
13	0	0	+
14	0	0	-
15	0	0	0

Several optical techniques were used during the study. Raman spectroscopy, Mie scattering, high-speed video imaging, and OH-chemiluminescence were all used in order to measure different jet characteristics.

The main technique, Raman spectroscopy was selected since it can measure the concentrations of all major species simultaneously. It is thereby possible to determine Φ in a volume of gas in one measurement. Raman spectroscopy has previously been used for measuring Φ in fuel sprays in various pressure chambers or combustion vessels, both as point and as line measurements (see e.g. [9,10,17,18]). It is an established technique and its theory is described in [19,20,21] or, more fundamentally, in [22]. Spectroscopic data can also be found in [23].

The only requirements for detecting multiple species with Raman scattering is that the signals from the different molecules have sufficient intensity and do not overlap too much spectrally, if one is to avoid more advanced computations and calibration strategies [24]. The Raman signal can then be expressed as

$$I_{Raman} = I_0 n \frac{\partial \sigma}{\partial \Omega} \Omega l \varepsilon \quad (3)$$

where I_0 is the laser intensity, n is the number density of a specific species (given by the pressure, temperature and composition), ε is a measurement constant, Ω is the collection solid angle determined by the optics, l is the length of the observed segment of gas and, finally, $\partial \sigma / \partial \Omega$ is the Raman cross section that varies for different species [20]. The Raman cross section, $\partial \sigma / \partial \Omega$, can be expressed in terms of the Raman shift and the Raman Strength (at least for diatomic molecules). For the major species in a combustion process these terms can be seen in Table 3 [20,23].

Table 3 Raman shifts and relative Raman strength for various molecules at RTP and 532 nm. [20,23]

Molecule	Raman shift (cm ⁻¹)	Relative Raman strength for 532 nm at RTP
N ₂	2331	1
O ₂	1556	1.41
Isooctane, CH	2903	--
H ₂ O	3652	1.96
CO ₂	1388(ν_1) / 1285(2 ν_2)	0.98 / 1.3

The Raman shift is the spectral distance between the laser wavelength and the Raman peak. The Raman strengths in Table 3 are given relative to the N₂ signal strength and for excitation with 532 nm radiation at room temperature and pressure (RTP).

Generally, the Raman strength varies with the laser frequency, ν_{laser} , as

$$I_{Raman} \propto (\nu_{laser} - \nu_{shift})^4 \quad (4)$$

Accordingly, the signal strength theoretically increases by a factor of 16 when changing the laser wavelength from 532 to 266 nm. However, the *relative* Raman signal strength can also be wavelength dependent. O_2 exhibits resonances that may increase the signal when using ultra violet (UV) lasers. E.g. with 266 nm radiation the relative cross section for O_2 is 2.0 instead of 1.41 [25].

For larger molecules, the Raman spectrum is more complicated. Isooctane, which was used in this study, was found to have at least six clearly identifiable peaks between 500 and 3500 cm^{-1} . The Raman strength of these peaks can vary with temperature and pressure as the relative population of the different vibration modes change [19]. These dependencies render it necessary to calibrate the Raman signal for the given conditions in the engine.

The major drawback with Raman spectroscopy is the low signal strength. A common way to increase the signal is to use very high laser energy, or using UV-lasers in order to increase the Raman cross section [26]. The laser beam also needs to be focused in the measurement region to increase the signal level. This leads to high fluence through the quartz liner around the combustion chamber, which can lead to optical damage. To circumvent this problem the current experiment employed a laser system that produced a train of eight pulses of 266 nm laser radiation. Each pulse thus had a peak power below the damage threshold of the quartz liner while the sum of the pulse train provided enough energy to give an acceptable signal level.

The presence of droplets or decomposed fuel in the measurement volume makes it impossible to define and measure a Φ value. Raman measurements in reacting jets must therefore be performed downstream of the liquid region and upstream of the reaction zone. To find suitable measurement positions, the liquid penetration length was measured using Mie scattering and the lift off length was measured using OH-chemiluminescence. It was found that there was not enough space for measurement between these two zones. In some cases reactions started at the jet periphery at a distance from the injector where there still occurred droplets in the spray. This is consistent with earlier studies [27,28].

Since it therefore was impossible to make the Raman measurements in reacting jets the engine was operated with isooctane to produce non-reacting jets. The same engine settings were used as during the emission measurements. Also the O_2 concentrations could be maintained as EGR was taken from an external source. The absence of combustion is expected to slightly affect the air entrainment into the jet. The flame itself is not expected to affect the air entrainment upstream of the

reaction zone. Previous research on a lifted flame shows that the air entrainment behaves as on a non-reacting jet up to the flame base and as on a reacting jet after the flame base [29]. As seen in EQ (2), however, the entrainment rate depends on the ambient density which is increased during combustion. Local ϕ -values are therefore expected to be somewhat lower in a reacting jet. Even if the absolute Φ -values measured in the non-reacting jets may be slightly higher than in reacting jets, the trends and main effects obtained in this investigation should still be relevant for reacting jets.

Using a laser wavelength of 266 nm can produce LIF, mainly from polyaromatic hydrocarbons (PAH) but also from O_2 in some cases. This may interfere with the Raman signal. Using non-reacting jets and keeping the fuel clean from fluorescent material from fuel lines etc., this problem is avoided.

The lift-off measurements using OH-chemiluminescence also has some complicating aspects. Natural luminescence from soot can be transmitted even through a narrowband UV interference filter. Care must be taken to avoid misinterpretation of the images, especially when the lift-off position is close to the bowl perimeter and the intense soot radiation there. To avoid this problem a camera equipped with a stereoscope was used that had a interference filter for OH-detection on one entrance and a neutral density (ND) filter on the other. This setup produced two simultaneous images of the combustion process that could be used to distinguish the much weaker OH-chemiluminescence from the natural luminescence. Regions in the images that show strong OH signal but no signal in the other image must be caused by OH-chemiluminescence. Such regions were found at the jet peripheries and closer to the nozzle than the natural luminescence; a clear indication of the lift off position.

EXPERIMENTAL SETUP

ENGINE SETUP - A Scania D12 heavy duty diesel engine, converted into an optically accessible single cylinder engine of Bowditch design, was used in this investigation. Details of the engine setup can be found in Table 4. A Cummins common-rail fuel injection system with solenoid valves was used along with two three-hole injectors with different orifice diameters; 100 μm and 140 μm . "EGR" was taken from an external diesel furnace for domestic heating. It was mixed with the inlet air and conditioned using a mechanical compressor and electric heater. This allowed independent control of inlet oxygen concentration, boost pressure and temperature.

Table 4 Engine properties.

Compression ratio, r_c [-]	15.6
Displacement volume [l/cylinder]	2.0
Bore [mm]	127
Stroke [mm]	154
IVC [CAD BTDC]	151
EVO [CAD ATDC]	146
Engine speed [rpm]	1200
Swirl number [-]	2.18
Fuel (non-reacting sprays)	100 % isooctane
Fuel (reacting sprays)	70% n-heptane 30% isooctane

The engine was operated at 6 bar indicated mean effective pressure IMEP and the TDC condition was matched to a realistic quarter load case. The combustion phasing was kept constant with the crank angle of 50 % completion of the heat release (CA50) at 11 CAD ATDC in order to achieve comparable conditions for all test cases. When the injection pressure was changed both the SOI and the energizing time of the injector had to be changed to achieve the same combustion phasing and amount of injected fuel, see Table 5.

Table 5 Fuel injection properties

	100 μ m injector		140 μ m injector	
Injection Pressure [bar]	SOI [CAD ATDC]	Energizing time [ms]	SOI [CAD ATDC]	Energizing time [ms]
1500	-22	3.2	-16	1.9
2000	-19	2.5	-11	1.6
2500	-15	1.9	-9	1.3

During emission tests the engine was fuelled with a mixture of 69% n-heptane, 30 % isooctane, and 1% of a transparent lubricant, Chevron Synfluid. The lubricant was used in order to ensure the function and lifetime of the fuel pump and the injector. This fuel mixture was chosen since it has a well known composition, as opposed to commercial diesel fuels, thus minimizing the risk of LIF interference from unknown species. The mixture has a cetane number similar to U.S. diesel. During the Raman and Mie measurements the engine was operated with non-reacting jets. These were obtained by using a blend of 99 % isooctane and 1 % of the lubricant.

OH-CHEMILUMINESCENCE - The lift-off length was measured using a Princeton PI-MAX2 CCD camera equipped with a stereoscope. The camera had a 1024 by 1024 CCD chip and was equipped with a B. Halle Nachfl. UV lens ($f_{\#} = 2$, $f = 100$ mm) and a stereoscope producing two images on the chip. The stereoscope was equipped with two filters. A narrowband interference filter was placed on one entrance to filter out the OH

chemiluminescence. It had a central transmittance wavelength of 310 nm, an indicated peak transmittance of 16.6 %, and a full width at half maximum (FWHM) bandwidth of 11.5 nm. An ND filter, OD 3, was placed on the other entrance to provide a signal level from the natural soot luminescence similar to that from the OH-chemiluminescence on the CCD. The exposure time was set to 68 μ s during the OH-chemiluminescence measurements.

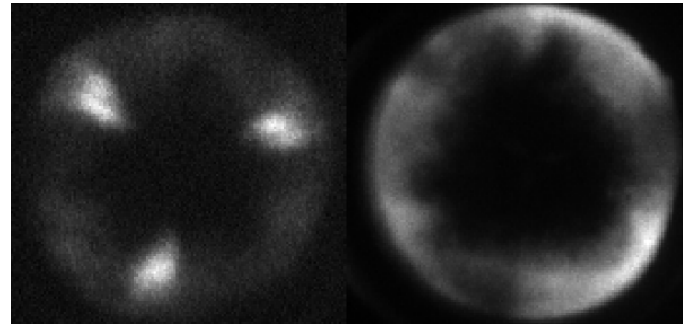


Figure 2 The left image shows the OH-chemiluminescence and the right image shows the natural chemiluminescence for the baseline case. The two images were captured on the same CCD chip simultaneously.

An example image from the OH-chemiluminescence measurements can be seen in Figure 2. The left part of this image shows the OH signal and the right part shows the natural chemiluminescence as seen through the ND-filter. The OH-chemiluminescence occurred well upstream of the natural luminescence. The relatively diffuse OH images were caused by the diluted operating condition, decreasing the flame temperature and thereby the OH signal. The lift-off length was determined by evaluating the averaged signal strength as a function of radial distance from the injector within a sector containing one spray. The radial position where this signal exceeded a certain threshold value was defined as the lift-off position. The threshold value was set to 3.5 % of the maximum intensity which was the lowest value that could be used due to background noise. Each mean lift-off position was evaluated from 99 single shot images. There was substantial variation on a cycle-to-cycle basis, with a standard deviation in the range of 1 to 1.5 mm. The OH-chemiluminescence, Raman and Mie measurements were all evaluated between 8 and 12 CAD ATDC, during the quasi-steady jet phase.

HIGH SPEED VIDEO IMAGING - The combustion chamber was also imaged using a high speed video system. A Phantom v 7.1 camera from Vision Research and a Hamamatsu high speed gated image intensifier were used. The system was equipped with a 105 mm $f_{\#} = 4.5$ UV-Nikkor lens from Nikon operated at $f_{\#} = 5.6$ and with the 310 nm interference filter described in the previous section. The high speed video system was used to investigate the position and the stability of the lifted flame. This was done in order to determine in what region the Φ -measurement should be performed and also to determine the quasi-steady phase of the