The Impact of Injection Timing on Mixture Preparation and Chemical Kinetics in Low-Temperature Diesel Combustion

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ABSTRACT

Mixture formation and the chemical kinetics of combustion are examined in an automotive diesel engine operating at 1500 rpm and a fuel quantity corresponding to 3 bar gross IMEP. Laser-induced fluorescence of a toluene fuel tracer is used to obtain quantitative in-cylinder distributions of the fuel-air equivalence ratio, and homogeneous reactor simulations employing detailed chemistry are used to examine the impact of kinetics.

With advanced combustion timing, losses in combustion efficiency and work output are found to be dominated by deficiencies in the mixture preparation process. With retarded injection, however, the chemical kinetics of combustion is the limiting factor. Trends in engine-out emissions are consistent with the measured mixture distributions and the results of the simulations.

INTRODUCTION

Low-temperature diesel combustion systems offer promise for reducing the in-cylinder formation of NO_x and particulates, thereby reducing the demands made on exhaust-gas after-treatment systems. These combustion systems can be problematic at low-load, however, where elevated emissions of UHC and CO can result in a significant fuel consumption penalty. Nonetheless, previous studies [1,2,3] have shown that there is an optimum injection timing, typically ~20–30° before TDC, that minimizes UHC and CO emissions and that corresponds closely to the optimum injection timing for best fuel economy.

Opat and co-workers [2] found that the increase in CO emissions with overly advanced injection timing correlates strongly with the mass of fuel injected directly into the squish volume. Multi-dimensional simulations further suggested that obtaining an appropriate split between the amount of fuel placed in the squish volume and in the bowl was a key to reduced CO emissions. With retarded timing, however, increased intake temperature caused a modest reduction in CO emissions, indicating that finite-rate kinetics could be important. Kook et al. [4] further argued that mixing was enhanced when fuel injected into the squish volume was forced back into the bowl by the squish flow. Thus, advancing injection to place more fuel into the squish volume could be beneficial, provided the amount of advance was not excessive. Lastly, Koci et al. [5] used speciated UHC measurements to investigate UHC emissions as injection timing is varied. They found that heavy UHCs ($C > 6$)

increase monotonically as injection is advanced, while the lighter UHCs correlate strongly with CO emissions and show a distinct minimum near the optimal injection timing. Koci et al. also show that, at the operating condition studied, the light UHC has a significant component associated with overly rich mixtures, as indicated by the C_2H_2 content.

Each of the above studies identified mixing processes as an important factor in determining the optimum injection timing. However, these conclusions were drawn solely from simulation and modeling results, or inferred from the behavior of the engine-out emissions. In this work we quantitatively measure the in-cylinder equivalence ratio (ϕ) distributions present at the start of combustion in order to gain more direct insight into the changes that occur in the mixture formation process as injection timing is varied. Moreover, we carefully evaluate the impact of injection timing on the chemical kinetics of combustion and show that both mixing processes and kinetics can have an important influence on the UHC and CO emissions.

ENGINE AND EXPERIMENT

ENGINE – An optically accessible diesel engine based on the GM 1.9 L serial production engine was used to obtain all of the measurements reported here. The specifications of the engine and injection system are provided in Table 1, and a schematic diagram of the engine is shown in Fig. 1. The fused-silica piston top incorporates a production-like bowl shape and valve pockets on the upper surface. Optical access into the

cylinder is provided by an extended piston and 25 mm high fused silica windows in the upper liner. The liner windows allow unobstructed optical access into the clearance volume even at TDC.

The major difference between the optical engine piston geometry and the production engine is in the volume of the top ring-land crevice, which is 3–4 times larger in the optical engine. Despite the larger crevice (and potential differences in combustion chamber surface temperatures), the optical engine has been shown to reproduce the emissions and combustion behavior of a similar all-metal engine [6].

The base fuel was a non-fluorescing mixture of 75% by volume *n*-heptane and 25% *iso*-octane. This blend matches the heat release and ignition delay of a US 2007 certification diesel fuel with a cetane number of 47 well. Previous work [3] has shown that the magnitude and trends with injection timing of UHC and CO emissions measured with this fuel blend are similar to those observed with diesel fuel. Toluene was added to the base fuel (0.5% by weight) as a fluorescent fuel tracer. Due to its thermal stability, its close match to the boiling point to the base fuel, and its well-characterized photophysics [7,8], toluene has been employed in several previous studies to measure local equivalence ratios and temperature, e.g. [9,10]. A solenoid-driven common-rail fuel injection system was used. Additional details describing the nozzle geometry are provided in Table 1.

OPERATING CONDITIONS – Toluene fluorescence is strongly quenched by O_2 ; accordingly, the engine was operated with a pure N_2 intake stream and combustion did not occur. The intake temperature and the mass flow rate of N_2 were selected, however, to match the near-TDC temperature and density of the 10% O_2 charge composition employed in our previous work. This matching allows comparison with measured engine emissions and with previous measurements of in-cylinder UHC distributions measured under combusting conditions [11]. The near-TDC thermodynamic conditions and other relevant operating parameters are listed in Table 2.

Three different injection timings were selected. The injection timing of -23.3° aTDC was near optimum for both UHC and CO emissions as well as fuel consumption. When the timing was advanced, the engine load fell rapidly; with an advance of only 4.5° to -27.7° , the load dropped from 3.0 to 2.4 bar. The performance deterior-

Table 1 Engine and fuel injection system specifications

Engine Geometry	
Bore / Stroke	82.0 / 90.4 mm
Geometric CR	16.7
Squish Height	0.88 mm
Injector specifications	
Injector	Bosch CRI2.2
Nozzle Type	Mini Sac (0.23 mm ³)
Holes / diameter	7 / 0.139 mm
Included Angle	149°
Hole geometry	KS1.5/86

Fig. 1 Schematic of the optically accessible diesel engine depicting the PLIF imaging configuration

ation was less rapid as timing was retarded. When injection was retarded by 10.8° to -12.5° , the load dropped to 2.8 bar.

PLIF DIAGNOSTIC – Toluene fluorescence was excited with a 266 nm, ~ 40 mJ/pulse laser sheet 0.5 mm thick, which entered the cylinder through the liner windows – as shown in Fig. 1. Fluorescence emissions were collected through the extended piston with a 105 mm, $f/4.5$ UV Nikkor lens equipped with a WG295 long-pass filter. Collected light was focused into an intensified CCD camera, which was gated for 250 ns. At each crank angle, 100 single-shot PLIF images were acquired. Single-shot laser pulse energies were measured for use in the data reduction process.

PLIF images were acquired at three horizontal planes, illustrated in Fig. 2. The upper plane bisected the clearance volume, and the two lower planes were fixed with respect to the piston bowl at locations where the bowl surface normal lay in the plane of the laser sheet.

To remove interferences from the PLIF images, background images were acquired at each crank angle with the laser running but without fuel injection. Calibration images were also obtained in a homogeneous mixture with approximately the same cylinder-averaged

Table 2 Details of the operating conditions

Operating Parameters	
Engine speed	1500 rpm
N_2 Charge $T_{\text{intake}} / P_{\text{intake}}$	300 [K] / 1.5 bar
Swirl ratio	2.2
Squish Height	0.88 mm
Motored TDC density*	21.1 [kg/m ³]
Motored TDC Temp.*	908 [K]
Injected fuel quantity	8.8 mg
Global $\phi^\dagger$	0.40
Injection pressure	860 bar
Start of Injection (SOI)	$-27.8, -23.3, -12.5^\circ\text{CA}$
Injection duration	5.4°CA (600 μs)

* based on GT-Power modeling of the induction and compression stroke

† assumes a 10% O_2 charge composition

Fig. 2 Location of the PLIF measurement planes. The piston position is shown at -17.5° aTDC. Darkened portions of the laser sheets correspond to imaged areas

equivalence ratio. The homogeneous mixture was created by 9 short injections made during the induction stroke.

Background-subtracted PLIF images were converted to equivalence ratio by normalizing by the calibration images, accounting for differences in laser energy, cylinder pressure and temperature, and for the temperature dependence of the toluene fluorescent yield. An iterative temperature correction, based on an assumption of adiabatic fuel-air mixing, was used. The equivalence ratio images were then corrected for the optical distortion incurred by viewing through the curved piston surfaces. Portions of the images where laser sheet interference or extreme distortion prevented quantitative measurements were replaced with a white mask.

Two principal sources of interference in the measurements cannot be removed by the background subtraction process. The first, associated with reflections of laser-induced fluorescence from combustion chamber surfaces, is most severe when regions of very low and very high ϕ co-exist within the plane of the laser sheet, and when the laser sheet is positioned close to the cylinder head (i.e., Plane 1). In this case, a ϕ as high as ~ 0.3 can be measured in regions between the jets where no fuel is expected. The second source of interference is associated with fluorescence arising from liquid fuel outside the plane of the laser sheet, which is excited by scattered laser light. Errors from this source are only significant early in the mixture preparation process. The thermal boundary layer along the head can also affect the accuracy, although this error is minimized by the normalization procedure described above.

Additional details describing the data acquisition, calibration, and image processing procedures can be found in references [12] and [13].

SIMULATIONS – Simulations of the oxidation kinetics were performed with CHEMKIN-PRO software, using the detailed kinetic mechanism for PRF mixtures described in [14]. The simulations were performed for a homogeneous, adiabatic mixture with the pressure constrained to follow the experimentally measured pressure. For each injection timing, the start of the simulation was chosen such that the ignition delay of $\phi = 1.2$ mixtures matched the measured ignition delay. Initial temperatures for each equivalence ratio were estimated from the adiabatic charge compression temperature assuming liquid fuel at an initial temperature of 90°C . UHC and the CO emissions indices were calculated from simulation predictions at 90° aTDC for each ϕ .

RESULTS

The cylinder pressure and apparent heat release rate

Fig. 3 Cylinder pressure and apparent heat release rate for each of the three injection timings.

characterizing the engine operation are shown in Fig. 3. The diamond symbols overlaid on the individual heat release curves designate the crank angle at which 10% of the total, cumulative apparent heat release has been released (B10). Open circles designate those crank angles closest to B10 at which PLIF images of the ϕ distributions were taken. Beyond B10, the ϕ distributions measured would not be typical of fired operation due to the absence of volume expansion and viscosity changes associated with heat release when the engine is operated with a pure N_2 intake charge.

Variation in SOI has a significant impact on the ignition delay, defined here as the time from SOI until B10. At the earliest injection timing, the ignition delay is 23° , and shortens to 20° and 15° for $\text{SOI} = -23.3^\circ$ and -12.5° , respectively. Accordingly, in addition to changes in the mixture preparation process caused by changes in the spray targeting there will also be changes associated with the longer ignition delay. Evidence of such changes in the mixture preparation process is given in Fig. 3 by the lower peak heat release rate observed with $\text{SOI} = -27.8^\circ$ than for $\text{SOI} = -23.3^\circ$, despite similar phasing and hence in-cylinder temperatures. More direct evidence of the changes that occur in the mixing process is provided by the PLIF images of equivalence ratio presented below.

In addition to the impact on ignition delay, SOI impacts the kinetics of the oxidation process during the entire combustion event, through differences in the magnitude and temporal evolution of the ambient pressure and temperature. One measure of the integrated effect of the combustion kinetics is provided by the predicted UHC and CO emissions index – shown in Fig. 4. To better compare the energy content associated by the UHC and CO emissions, we have multiplied the emissions index by the respective lower heating value (UHC is assumed to have the heating value of the fuel) and normalized by the heating value of the fuel.

Figure 4 clearly shows that within the range of injection timings investigated, SOI has very little impact on the emissions of UHC and CO stemming from rich mixtures; emissions from these mixtures result from a deficit in O_2 , not limited kinetic rates. However, very large differences are seen for lean mixtures. With earlier injection, there is a greater amount of time available to complete reaction, and compressive heating helps amplify the temperature increase associated with early heat release. Consequently, leaner mixtures are able to

Fig. 4 Predicted energy content of UHC and CO emissions for the combustion of homogeneous mixtures in an environment following the experimentally measured cylinder pressure

complete combustion. In addition, for very lean mixtures ($\phi \leq 0.3$), the energy content in the UHC emissions is expected to be considerably larger than the energy content in the CO emissions. Combustion of moderately rich mixtures ($\phi \leq 2$), on the other hand, provide CO emissions with a greater energy content than the UHC emissions. We therefore expect that with longer ignition delay, resulting in an increase in lean mixture and a decrease in rich mixture, the energy content of UHC emissions will increase more rapidly than that of CO emissions. Finally, with retarded SOI, there is a relatively narrow region of equivalence ratios, $0.75 \leq \phi \leq 1$, where emissions of CO and UHC are low. While further mixing during the combustion process will likely reduce or eliminate emissions stemming from rich mixtures, mixtures formed during the ignition delay period with an equivalence ratio less than ~ 0.75 will almost certainly result in UHC and CO emissions.

With the insight provided from the heat release analysis and the simulation predictions, considerable understanding of the mixture formation processes can be inferred from the measured engine-out emissions, which are shown in Fig. 5:

- 1) The increase in UHC emissions at advanced injection timing is inconsistent with the predicted UHC emissions trends, which indicate that advanced injection will favor oxidation if the mixture distributions formed are equivalent. Accordingly, we conclude that changes in the mixture distribution is responsible for the increased emissions—either through formation of a greater quantity of very lean mixtures during the extended ignition delay or through increased rich mixtures and crevice hydrocarbons associated with injecting a greater amount of fuel into the squish volume.
- 2) The increase in CO emissions observed as injection is advanced and ignition delay lengthened, suggests that rich mixtures are not the dominant source of CO emissions, at least at the most retarded injection timings. We have reached a similar conclusion from

Fig. 5 Engine-out emissions measured as a function of injection timing

our examination of the variation in emissions with engine load in our previous work [11]. However, at the earliest injection timings, rich mixture in the squish volume or fuel in the ring-land crevices may be contributing to the rapid rise in CO emissions.

- 3) The decrease in NO_x emissions as injection is advanced is almost certainly associated with the combustion of a smaller quantity of mixture in near-stoichiometric premixed combustion or in mixing-controlled combustion. The leveling or slight increase in NO_x at the most advanced injection timing is likely associated with rich mixture created by injection of fuel directly into the squish volume.

MEAN EQUIVALENCE RATIO DISTRIBUTIONS –

Our emphasis in this paper is on quantifying the mixture distribution near the start of combustion, B10. We accordingly present the mean images of the in-cylinder ϕ distributions referenced in time to B10 for each SOI investigated.

Figure 6 shows the spatial distributions of ϕ measured 10° prior to B10 (B10- 10°). With the most

Fig. 6 Equivalence ratio distributions measured 10° before the start of combustion

advanced injection timing, the fuel jets have penetrated well into the squish volume and are likely to be in contact with the cylinder wall and the ring-land crevice. Similarly, the jets have penetrated deep into the bowl, traversed the bowl floor, and are rising up against the bowl pip. The peak equivalence ratios observed in the bowl are considerably lower than those observed in the squish volume, but are still fuel-rich. In contrast, the mixture in the bowl rim plane and near the cylinder head above the bowl is generally fuel lean, and it is already apparent that over-lean mixtures that will be unlikely to complete combustion have been formed.

With $\text{SOI} = -23.3^\circ$, however, rich mixture is still found in the central regions of the cylinder, in both planes 1 and 2. Like the advanced injection timing, the fuel jets have penetrated well into the squish volume, but have not reached the cylinder wall and are less broadly dispersed azimuthally. Within the bowl, the fuel-rich jets are seen only against the outer bowl wall.

At the most retarded injection timing the fuel injection process is still on-going, although the end of injection is being approached. While the jets have impacted the bowl rim, they have not yet penetrated into the visible portion of the squish volume. The heads of the jets are seen to just be entering the bowl plane; however, the faint ghosts of fuel observed trailing toward the central pip, and the brighter spots near the pip, are artifacts of reflections and fluorescence from out-of-plane liquid fuel and should be disregarded.

Later, at $\text{B10}-5^\circ$ (Fig. 7), the mixture distributions observed at the advanced timing within the squish volume are quite similar to those seen at $\text{B10}-10^\circ$, though the heads of the jets are somewhat leaner. In the central region of the cylinder, in both planes 1 and 2, lean mixture that will likely contribute to UHC and CO emissions continues to be observed; in this region mixing processes have almost completely removed any semblance of a discrete fuel jet structure. Likewise, the mixture within the bowl is becoming more homogeneous, but is characterized by more fuel-rich mixtures.

At the near optimal injection timing of -23.3° , the jets have penetrated only slightly further into the squish volume than was seen at $\text{B10}-10^\circ$, and are unlikely to be making significant contact with the cylinder wall. Like the more advanced injection timing, we see over-lean mixture, which will be unlikely to complete combustion, forming in the central region of the cylinder in the upper two planes. In the lower bowl plane the fuel distribution is similar to that seen with the more advanced injection 5° earlier in Fig. 6: the fuel jets have traversed the bowl floor are now rising up against the bowl pip.

Finally, with retarded injection, there is very little penetration of the fuel jets into the squish volume even though 10° have passed since the start of injection. In contrast, with $\text{SOI}=-23.3^\circ$, significant penetration into the squish volume was seen in Fig. 6 only 8.3° after SOI, and with $\text{SOI}=-27.8^\circ$ the jets had penetrated to nearly the cylinder wall just 7.8° after SOI. Mixture deep in the bowl, where most of the fuel has been directed, is considerably richer than is observed in the two earlier injection cases. As will be seen below, this bowl mixture remains fuel-rich through the start-of-combustion.

Equivalence ratio distributions measured at the

Fig. 7 Equivalence ratio distributions measured 5° before the start of combustion

Fig. 8 Equivalence ratio distributions measured at B10, the start of combustion

start-of-combustion (B10) are shown in Fig. 8. Clear trends are seen in the mixture distribution within the squish volume as injection is retarded: 1) there is less penetration and a lower probability of fuel entering the ring-land crevice, 2) there is less rich mixture in the heads of the jets, and 3) there is less overly lean mixture between the heads of the jets. Likewise, in the bowl rim plane, there are clear trends towards a less homogeneous mixture with less overly lean mixture as injection is retarded. These trends also hold in plane 3 within the bowl, but in this plane the amount of rich mixture increases strongly with more retarded injection.

The impact of the ϕ distributions on UHC and CO emissions can be estimated by multiplying the fuel mass distributions at B10 by the UHC and CO yields shown in

Fig.9 Estimated UHC and CO emissions derived from the measured ϕ distributions and the predicted CO and UHC yield shown in Fig. 4

Fig. 4. The fuel mass distributions are found by summing the mass of fuel at each equivalence ratio over all pixels (i, j) in the images of Fig.8:

$$m_{\text{fuel}}(\phi) = \sum_j \sum_i m_{\text{fuel},i,j}(\phi) = \sum_j \sum_i \phi_{i,j} m_{\text{charge},i,j} \left(\frac{m_{\text{fuel}}}{m_{\text{charge}}} \right)_{\text{stoich}} \quad (1)$$

The results, shown in Fig. 9, are the expected UHC and CO emissions as a function of equivalence ratio, assuming no further mixing occurs as combustion proceeds. Important points to note from Fig. 9 are:

- 1) UHC is dominated by lean mixture and increases significantly as injection is retarded, despite the shorter ignition delay and the smaller quantity of over-lean mixture seen in Fig. 8. This is due to the significantly greater UHC yield seen in Fig. 4 for retarded injection, where kinetic effects clearly limit the combustion process.
- 2) At the most advanced injection timing, the predicted UHC emissions are small – contrary to the emissions measurements shown in Fig. 5. The increase in measured emissions at advanced timing is therefore almost certainly due to crevice UHC, though rich mixture sources are also becoming important. A high probability of crevice sources of UHC is clearly indicated by the ϕ distributions shown in Figs. 6-8.
- 3) The predicted CO emissions decrease with retarded injection, like the measured emissions. CO emissions potentially arising from rich mixtures are minimized near the optimal injection timing.
- 4) In general, for all injection timings, UHC and CO emissions are dominated by lean mixture in the upper-regions of the combustion chamber.

SUMMARY AND CONCLUSIONS

Fuel-air equivalence ratio distributions measured in a light-duty diesel engine using a fuel tracer based LIF technique and homogeneous reactor simulations employing detailed kinetics are used to clarify the impact of injection timing on sources of UHC and CO in a low-temperature diesel operating condition.

The results indicate both CO and UHC emissions arise mainly from lean mixtures in the upper portion of the cylinder. Increased UHC at overly advanced injection timing is largely due to increased crevice UHC, while the increase at overly retarded timing is due to finite rate kinetics of combustion. CO emissions decrease as injection timing is retarded due to reduced formation of over-lean mixture. With overly advanced or retarded timing there is increased probability that CO emissions also stem from rich mixture sources.

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