

UHC and CO Emissions Sources from a Light-Duty Diesel Engine Undergoing Dilution-Controlled Low-Temperature Combustion

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ABSTRACT

Unburned hydrocarbon (UHC) and carbon monoxide (CO) emission sources are examined in an optical, light-duty diesel engine operating under low load and engine speed, while employing a highly dilute, partially premixed low-temperature combustion (LTC) strategy. The impact of engine load and charge dilution on the UHC and CO sources is also evaluated. The progression of in-cylinder mixing and combustion processes is studied using ultraviolet planar laser-induced fluorescence (UV PLIF) to measure the spatial distributions of liquid- and vapor-phase hydrocarbon. A separate, deep-UV LIF technique is used to examine the clearance volume spatial distribution and composition of late-cycle UHC and CO. Homogeneous reactor simulations, utilizing detailed chemical kinetics and constrained by the measured cylinder pressure, are used to examine the impact of charge dilution and initial stoichiometry on oxidation behavior. The measured distributions are also compared to multidimensional simulation results and with engine-out emissions measurements.

Homogeneous reactor simulations show that increased dilution leads to a narrower equivalence ratio (ϕ) range that allows for acceptable UHC and CO oxidation. As dilution increases, the increased charge-fuel mass ratio

for a given ϕ amplifies the impact of a reduced rich-limit ϕ for acceptable UHC oxidation, since a greater fraction of the fuel is embedded in rich mixture. In-cylinder UHC and CO imaging highlights the differences that changes in dilution and load have on the three main UHC source regions: 1) The cylinder center region contains intense near-injector fluorescence indicative of late-cycle fuel addition, while diffuse fluorescence is present from UHC and CO that is embedded in the surrounding fuel-lean bulk gases; 2) Within the bowl and central clearance volume, a rich mixture plume that exits the piston bowl is the dominant source of predicted UHC and CO, but is not observed experimentally; 3) Squish volume UHC and CO principally results from the partial oxidation of lean mixture, although UHC from piston top fuel films and crevice flows is also observed.

INTRODUCTION

In the effort to improve fuel economy and minimize green house gas emissions, compression ignition (i.e. diesel) combustion strategies are currently being aggressively pursued. Increasingly stringent regulation of nitrogen oxide (NO_x) and particulate matter (PM) emissions, however, generally requires engine-out exhaust aftertreatment which may adversely affect fuel economy and increase overall vehicle cost. To reduce

the cost and complexity of aftertreatment systems several low-temperature combustion (LTC) strategies have been devised as a way to reduce the in-cylinder formation of NO_x and soot—a significant component of PM.

One LTC variant, partially premixed compression ignition (PPCI), has been actively investigated [1-6]. PPCI promotes lower combustion temperatures and enhanced pre-combustion fuel/air mixing through a combination of moderate swirl, low compression ratio, heavy charge dilution by exhaust gas recirculation (EGR), and an advanced start-of-injection (SOI). The resulting reductions in soot and NO_x emissions are offset, however, by decreased fuel efficiency and increased UHC and CO emissions, particularly at lower loads. Understanding and mitigating the sources of these emissions and the associated efficiency loss is essential for the viability of engines employing PPCI combustion.

Emissions of UHC and CO for conventional diesel combustion, although low, are generally attributed to incomplete bulk-gas oxidation [7] from either overly-lean regions that are easily quenched during expansion or from overly-rich regions with insufficient O_2 [8, 9]. For PPCI combustion, UHC and CO emissions are more significant, and generally track each other as the operating conditions are changed [5]. Previous studies performed in light-duty engines [5, 6, 10] have observed decreased CO emissions with increased ignition delay and injection pressure, and a negligible impact with varying intake temperature—evidence of CO emissions dominated by rich mixture. Light load (1 bar IMEP) UHC emissions, however, have been significantly reduced through increased charge temperature [11]—behavior indicative of overly-lean emission sources that are limited by chemical reaction rates.

For PPCI combustion, UHC and CO sources not typically considered in conventional diesel operation such as wall and crevice quench layers, fuel introduced late in the cycle either from nozzle dribble or needle-bounce-induced secondary injections, and flash-boiling of piston surface fuel films [7, 12-15] may contribute. Misfire has also been suggested as a probable source, although low cycle-to-cycle fluctuations in UHC emissions [16] suggest the contribution from misfire is negligible. The relative contribution from each UHC source on overall emissions is dependent upon engine operating conditions, combustion chamber geometry, and fuel injection characteristics.

In a previous investigation of UHC sources for a PPCI combustion scheme using the same engine studied here, the impact of injection timing on UHC sources was examined [12]. A highly dilute (10% $[\text{O}_2]$), moderately boosted (1.5 bar intake pressure), lower-load (3.0 bar IMEP) operating condition was examined. Three main regions of UHC were identified:

The cylinder center and near-injector region – Although evidence of lean mixture UHC, possibly due to excessive

ambient entrainment at the end of injection [17], was observed near the cylinder center, much of the UHC in this region appears to originate from partially-reacted liquid- and vapor-phase fuel leaving the injector late in the cycle.

The bowl and central clearance volume – The predictions of multi-dimensional simulations indicate that most of the engine-out UHC originates from under-mixed fuel within this region. Experimentally, however, UHC within this region is observed only infrequently.

The squish volume – Squish volume UHC resulting from piston-top films and ring-land crevice outflows was observed with maximum brake torque (MBT) and more advanced injection timing. With retarded injection timing, UHC within the squish volume was dominated by lean, low-temperature mixture.

To clarify the composition of the identified UHC sources, changes to chemical reaction rates are induced by variations in charge mass specific heat, combustion temperature, and mixture stoichiometry. This is achieved by fixing SOI and varying either intake charge dilution or engine load about the baseline operating condition. The impact of these processes on CO emission sources is examined as well. Direct in-cylinder visualization of UHC spatial distributions is performed via ultraviolet planar laser induced fluorescence (UV PLIF). Deep-UV PLIF is also utilized to visualize the late-cycle CO distribution and to characterize the composition of late-cycle UHC. Results from both homogeneous reactor simulations (simplified mixing but detailed chemistry) and multidimensional simulations (detailed mixing with simplified chemistry) are compared with the experimental results and used to help interpret the data.

ENGINE

The experiments were performed in a single-cylinder, direct-injection (DI), optically-accessible research engine, incorporating a production 4-cylinder General Motors 1.9L cylinder head with a Bosch CRI2.2 injector vertically mounted in the cylinder-center. Cylinder pressure was monitored using a Kistler 6125B quartz pressure transducer mounted in the glow plug position, and used to compute indicated mean effective pressure (IMEP) and apparent heat release rate (AHRR). The engine geometry and fuel injector characteristics are summarized in Table 1.

Although the piston-top was constructed from fused silica, the geometric characteristics of a typical production engine were preserved, including the reentrant bowl design, crevice width, and the piston-crown valve cutouts. The piston bowl geometry is illustrated in Fig. 1. Compared with a production piston, the only major design change is the lower position of the compression rings, which increases the ring-land crevice volume by 3–4 times, potentially influencing UHC and CO emissions that stem from this region. Nonetheless, because the crevice width is equivalent to what would be

Table 1 Engine and injection characteristics for all operating conditions, where conditions in bold represent the baseline.

Engine Characteristics: GM 1.9 L	
Bore / Stroke	82.0 / 90.4 [mm]
Displacement	477 [cm ³]
Load	1.5, 3.0 , 4.5 [bar]
SOI _{command}	-26.6 [°CA [†]]
SOI	-23.1 [°CA]
[O ₂]	9, 10 , 15 [%]
Engine Speed	1500 [rpm]
T _{intake}	98, 97 , 89 [°C]
P _{intake}	1.5 [bar]
CR (Geometric / Effective)	16.7 / 14.0
Swirl Ratio:	2.2
Injector Characteristics: Bosch CRI2.2	
Type / Sac Volume	Mini Sac / 0.23 [mm ³]
Holes num. / nozzle diam.	7 / d = 0.14 [mm]
Included Angle:	149°
Rail Pressure:	860 [bar]
Fueling Rate:	8.8 [mg/inj]
Fuel / Cetane #	US #2 Diesel / 43

[†] Crank angles given in this paper refer to TDC compression

found in a typical production engine (Fig. 1) and the cylinder is sealed using two gapless compression rings, minimal blow-by is expected. Although the 16.7 geometric compression ratio was maintained, an effective compression ratio of 14.0 more closely matches cylinder pressures and combustion behavior predicted by a one-dimensional engine simulation model. The change in compression ratio has previously been attributed to increased heat-loss resulting from the larger crevice volume [16]. Three standard grade fused-silica windows have been installed in the upper cylinder-liner, both for admitting laser radiation into the cylinder and viewing the resulting fluorescence. Like the larger ring-land crevice, the lower thermal conductivity of the fused-silica windows and piston-top may impact UHC and CO emissions by introducing differences in surface temperatures from those present in a production engine, possibly affecting fuel film vaporization and oxidation processes near the walls. Nevertheless, the UHC and CO emissions trends measured in a conventional single-cylinder test engine are well-captured [18].

OPERATING CONDITIONS

Emissions of UHC and CO in LTC engines typically are most problematic at lower loads and oxygen concentrations ([O₂]). Thus, we focus on the same highly dilute (10% [O₂]), lower-load (3.0 bar IMEP), moderately boosted (1.5 bar intake pressure) baseline operating condition studied previously [12]. The selection of this operating condition was based upon engine performance and emissions data acquired over a wide range of dilution levels, injection timings, and intake pressures [19]. At the selected baseline conditions, adequate

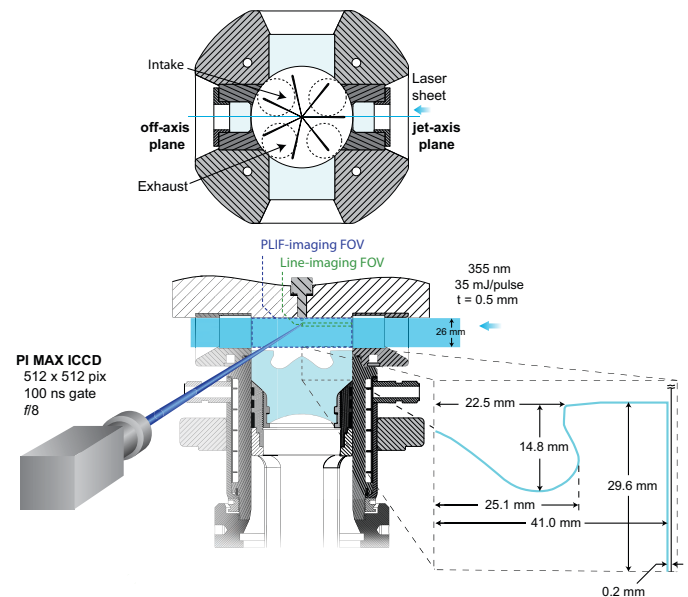


Figure 1 Cross-section of the optical engine and schematic representation of the experimental set-up for 2-D PLIF imaging of UHC. For deep-UV LIF line-imaging, the collected light was dispersed through a spectrometer. A cross-section of the piston bowl geometry is also included.

combustion efficiency (~98%) was obtained despite elevated UHC and CO emissions relative to higher [O₂], as shown in Fig. 2. By plotting UHC and CO emissions as their normalized heating value, CO emissions can be seen to dominate the efficiency loss. For the present study, the mixture composition of the UHC and CO sources was characterized by fixing injection timing and varying either charge dilution (9% or 15% [O₂]) or engine load (1.5 or 4.5 bar IMEP) about the baseline condition, thereby restricting changes in emissions to differences in charge mass specific heat, combustion temperature, or mixture stoichiometry. All operating conditions are summarized in Table 1.

The engine was skip-fired, with one fuel injection event every fifth cycle. Skip-firing helps maintain realistic quartz surface temperatures and has the added benefit that it prolongs the lifespan of fragile optical pistons. A consistent engine thermal state between tests was

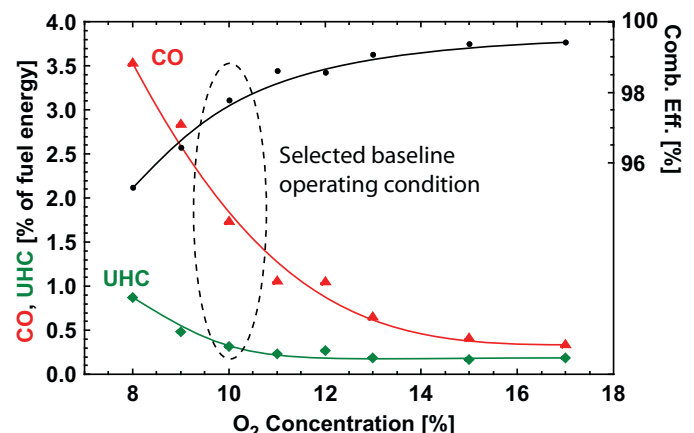


Figure 2 Emissions and combustion efficiency as a function of dilution at MBT timing (reproduced from [12]).

maintained by following an eight-minute operating schedule. At the beginning of the schedule, the engine was briefly motored for 100 seconds to stabilize intake plenum pressures. The engine was then skip-fired for an additional 2 minutes. To ensure that combustion chamber surfaces were sufficiently preheated, measurement acquisition began 75 seconds after the start of skip-firing. Once the measurements were complete, the engine was stopped and allowed to cool for the remaining duration of the eight-minute cycle. During the cool-down period, any accumulated soot or fuel films were cleaned from the optical surfaces before beginning the next run.

Due to the skip-fired operation of the engine, simulated EGR was necessary to obtain the desired intake $[O_2]$. The intake charge was diluted with N_2 and CO_2 in proportions that matched the equivalent real exhaust gas specific heat ratio (at 600 K), while maintaining a

Table 2 Mixture mass fractions and charge-to-fuel mass ratio for each test condition.

$[O_2]$	Air	N_2	CO_2	Charge/Fuel Mass ratio
9%	0.413	0.436	0.150	36.15
10%	0.460	0.402	0.138	32.45
15%	0.701	0.222	0.077	21.30

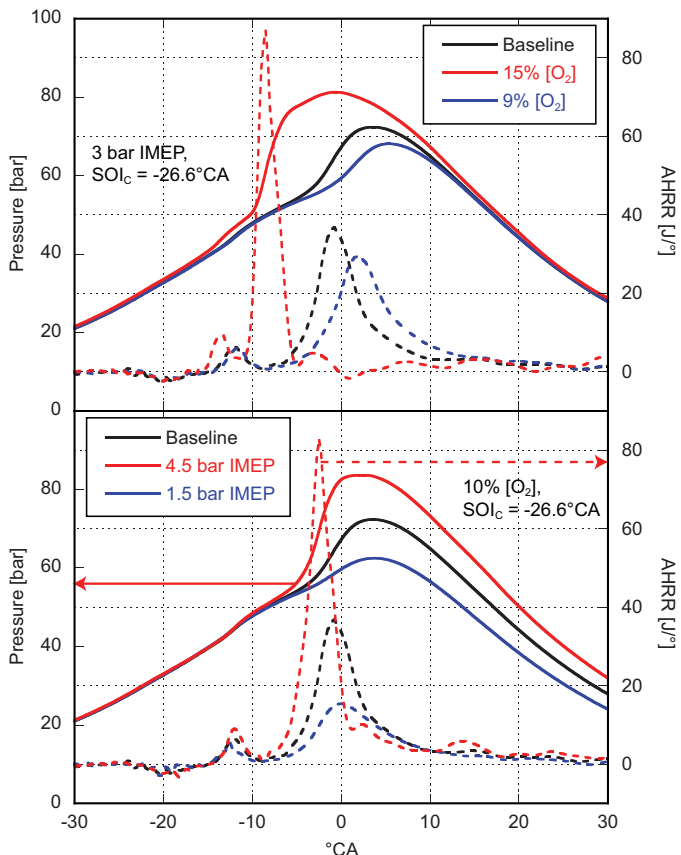


Figure 3 Characteristic cylinder pressure and heat-release traces for all operating conditions. Note that only the baseline operating condition injection timing is MBT.

constant intake mass flow rate (8.9 g/s). For each $[O_2]$, the intake temperature was varied such that the top-dead-center (TDC) temperature and density were constant. The intake charge mass fraction for each species and the stoichiometric charge-fuel mass ratio at each $[O_2]$ are summarized in Table 2. Characteristic pressure and apparent heat release rate (AHRR) traces for each condition are displayed in Fig. 3.

EXPERIMENTS

EMISSIONS EQUIPMENT – Engine-out UHC emissions were measured using a California Analytical Instruments flame ionization detector (600 MHFID), with a 0–1000 ppm (C1) measurement range. A calibration of the analyzer was performed using a 1000 ppm methane span gas. An exhaust plenum heater and heated sampling line and filter were used to prevent condensation within the exhaust. Emissions of CO were measured by a California Analytical Instruments 300 Nondispersive Infrared (NDIR) Gas Analyzer, with a 0–6000 ppm measurement range, after removing water and hydrocarbons in a condenser.

UHC UV PLANAR LASER INDUCED FLUORESCENCE Formaldehyde (CH_2O), poly-aromatic hydrocarbon (PAH), and parent fuel fluorescence was excited by a 25 mJ pulse from the third harmonic (355 nm) of a Nd-YAG laser (Spectra-Physics Pro-290). In over-lean mixtures that fail to oxidize completely ($\phi \leq 0.3$), either parent fuel compounds or CH_2O are likely to be present and thus detected by the PLIF diagnostic. Likewise, for the combustion of mixtures with $\phi \geq 2$, PAH formation is anticipated and UHC stemming from these very rich mixtures is also likely to be detected. Simulations of diesel combustion (e.g. [20]) indicate, however, that for moderately rich equivalence ratios ($1 < \phi < 2$), the combustion products likely contain almost no CH_2O , PAH, or other compounds that can be excited by 355 nm laser radiation. Thus, this UV PLIF diagnostic may be unable to image potentially significant sources of bulk-gas UHC.

A combination of spherical and cylindrical optics was used to form the laser beam into a sheet roughly 30 mm high and 500 μm thick, with an estimated $\pm 25 \mu m$ thickness variation throughout the cylinder. The vertical laser sheet entered the cylinder through the right-hand liner window (Fig. 1), and was aligned with the axis of one of the 7 fuel jets. For future reference, the phrase “jet-axis side” refers to the right-hand side of the images, while the “off-axis side” refers to the left-hand side where the laser sheet bisects the angle between two fuel sprays.

Images were obtained using a Roper Scientific PI-Max intensified camera, employing the maximum intensifier gain and a 100 ns camera gate. A balance between image focus through the curved bowl walls and light collection was achieved by using an aperture setting of $f/8$. At each crank-angle, 50 single-frame images were acquired. Spurious background signal from

the windows and injector tip was eliminated by subtracting a background image obtained 70 s into the motored portion of the operating schedule, approximately 145 s before the fired data were acquired. Large laser sheet irradiance variations, generated by refraction and reflections from the piston surfaces, were compensated for by performing a flatfield correction. Flatfield PLIF images were separately obtained by seeding the intake charge with 3000 ppm of formaldehyde, produced by introducing vapor from a 10% formalin solution (3.7% CH₂O by volume), and imaging fluorescence while the engine was motored. The signal-to-noise ratio of the flatfield images was ~8, more than sufficient for the desired qualitative spatial distributions of UHC. Run-to-run variations in laser energy were accounted for by normalizing the image intensity by the laser energy, measured using a Coherent J4-09 pyroelectric detector. The laser sheet was partially blocked by the bowl pip and injector tip, restricting off-axis imaging in the lower piston bowl and upper 2 mm of the clearance volume. Results in these regions should thus be interpreted with caution.

Optical image distortion in the clearance and bowl volumes resulting from the curved liner windows and piston bowl necessitated separate, piecewise-linear distortion corrections [21] derived from images of illuminated calibration grids. While clearance volume distortion is due solely to the upper liner windows, requiring only a single distortion correction, unique bowl corrections were necessary at each crank-angle. Distortion corrected clearance and bowl volume images were then recombined at the piston crown to form an image of the entire combustion chamber cross-section. Image noise was reduced using the combination of a 3 x 3 median filter and light (5 x 5) Gaussian smoothing filter ($2\sigma = 1.6$ pixels, corresponding to ~0.1 mm).

DEEP-UV UHC AND CO LIF – The deep-UV, 1-D line imaging LIF technique was similar to the method described by Kim et al. [22], and was used to characterize the late-cycle distribution of CO and composition of UHC. Fluorescence from UHC and CO was excited from a deep-UV laser beam generated by an optical parametric oscillator (Spectra-Physics MOPO 730) tuned to 230.1 nm, with typical pulse energies near 15 mJ. The beam was focused in the cylinder using a cylindrical lens ($f = 1000$ mm), resulting in a laser sheet width of approximately 500 μ m. At the excitation wavelength, CO LIF resulted from two-photon excitation of the $B^1\Sigma^+ \leftarrow X^1\Sigma^+$ transition, with emission in the $B^1\Sigma^+ \rightarrow A^1\Pi$ system occurring between 440 and 730 nm. The excitation wavelength also promoted C₂ ($d^3\Pi \rightarrow a^3\Pi$) Swan band fluorescence, emitting between 420 and 520 nm. The C₂ fluorescence is expected to result primarily from laser-induced fragmentation fluorescence (LIFF) of acetylene (C₂H₂), the vinyl radical (C₂H₃), butadiene (C₄H₆), and other combustion intermediates present in both lean and rich mixtures. For rich mixtures C₂H₂ is also expected in the product gases. Additionally, PAH fluorescence from smaller PAH molecules, which are relatively insensitive to the 355 nm PLIF wavelength, are

expected to be excited with the deep-UV laser. More complete spectroscopic details can be found elsewhere [23-28].

To reduce interference from the injector tip and piston surface, only a 3.4 mm high region of the sheet was admitted into the cylinder via 20 mm diameter cylindrical windows. These windows replaced the larger, side-mounted windows in the upper cylinder liner employed for the PLIF measurements, as shown in the upper portion of Fig. 1. The sheet position was adjusted daily to ensure the most intense portion of the sheet was imaged. Damage to the window surfaces by the laser pulses was an ongoing problem, which occurred after only a few thousand shots. To extend the usable window lifespan, a laser shutter was installed to prevent laser strikes when measurements were not acquired. In addition, more optically durable ArF grade fused silica windows were used for admitting laser radiation, while etched portions of the window were rotated out of the beam path between runs. To avoid laser damage to the quartz piston crown, a titanium piston crown was used which limited measurements to within the clearance volume.

Fluorescence was collected through the larger, standard grade fused-silica window by a 180 mm focal length lens and focused into an $f/4$, 1/4-meter spectrograph (SPEX 270M) equipped with a 384 x 576 pixel intensified CCD detector (Princeton Instruments ICCD-576E) controlled by a Princeton Instruments ST-138 controller and gated at 100 ns by a PG-200 high-voltage pulse generator. A 400 groove/mm grating provided a spectral range between 394–510 nm on the detector and—with a 0.5 mm entrance slit height—a spectral resolution of 5.3 nm. The resulting 1-D “line images” contained spectrally dispersed information along the cylinder radial axis.

Fluorescence imaging was impeded early in the expansion stroke due to laser sheet blockage by the 20 mm laser window mounts and by piston crown vignetting. The first crank-angle at which measurements were obtained was 30°CA, at two separate measurement heights centered 2.9 and 6.0 mm below the head. For each measurement, 50 spectrally-resolved images were integrated on the detector of the spectrograph. To examine the evolution of the spatial distribution of UHC and CO, measurements were also obtained at 50°CA at heights of 2.9, 10.4, and 17.9 mm below the head. Flatfield measurements, used to account for vignetting by the piston and combustion chamber walls, were obtained at the same heights and crank-angles by seeding a uniform concentration (3000 ppm) of CO into the intake charge and motoring the engine.

During post-processing, image noise was removed by applying a 3 x 3 pixel median filter and a 13 x 13 Gaussian smoothing filter ($2\sigma = 4.8$ pixels, corresponding to ~0.5 mm and ~1 nm along the spatial and spectral axes, respectively). Background signal was removed from each fired-cycle image by subtracting its

corresponding background image, obtained in a manner similar to that described for the PLIF diagnostic technique. An image of a calibration target was used to define 13 spatial bins, each 3 mm wide, spanning a radial distance from the cylinder centerline to within 2 mm of the bore wall. A spectrum characterizing the measured LIF emissions within each spatial bin was generated by integrating the intensity of the background-corrected images at a given wavelength over all pixels within the bin.

The spectral region of greatest interest lies between 445 and 495 nm, where two CO transitions (centered near 450 and 483 nm) and a group of C₂ Swan band transitions, centered at about 470 nm, exist on top of a broadband continuum attributed to PAH fluorescence. To separate the CO and C₂ fluorescence, we have improved on the method employed by Kim et al. [22], by locally modeling the spectrum as a superposition of a linear background (PAH) and three Gaussian functions centered on the three CO and C₂ transitions. A fourth Gaussian function accounting for elastic scattering from the MOPO fundamental beam (centered at 460.2 nm) was also employed, but was usually unnecessary since most of the elastically scattered light was removed by the background subtraction. A least-square-error minimization procedure was then employed to determine the best fit coefficients to the linear background and to the amplitude, center wavelength, and full width at half maximum (FWHM) of each Gaussian function. An example of the fit achieved between the measured and modeled spectrum, along with the individual Gaussian functions fit to both the fired and flatfield images, is shown in Fig. 4.

Raw CO and C₂ signal levels were determined analytically from the parameters characterizing each Gaussian function, and the raw PAH signal level was estimated as the integrated spectrum less the raw CO and C₂ signals. Since CO LIF is a two-photon process, the raw signals were normalized by the square of the measured average laser pulse energy. Quadratic scaling was also applied to the C₂ signal, assuming a partially

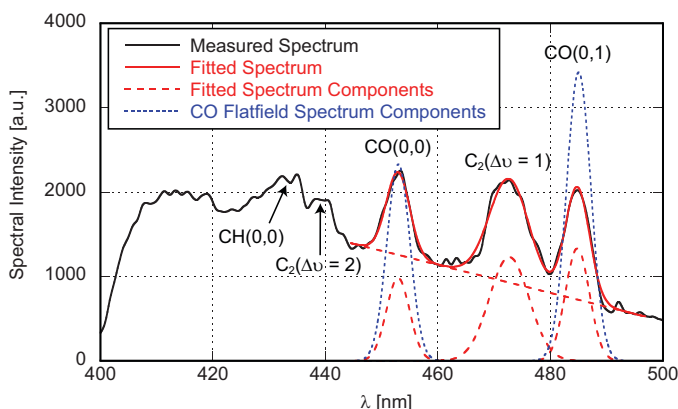


Figure 4 A sample spectrum, obtained 6.0 mm below the head at 30°CA, showing measured CO, CH and C₂ transitions along with the estimated PAH background and Gaussian fits to the spectra between 445 and 495 nm. CO signals derived from flatfield images are also shown for comparison.

saturated 3-photon LIF process [27]. PAH fluorescence, however, is linearly proportional to the irradiance; hence, the signal was normalized by the first power of the laser energy. Finally, to account for vignetting, fired-cycle signals were normalized by the corresponding signals obtained from the flatfield images.

Because the data were obtained at multiple measurement heights, the CO and UHC spatial information is available in two dimensions. To aid in the visual interpretation of the data, an approximate 2-D cycle-averaged spatial distribution was created by applying a spline fit to the measured data points and extrapolating to the combustion chamber walls using a constant slope boundary condition.

PARTICLE IMAGE VELOCIMETRY – Mean velocity fields, measured using particle image velocimetry (PIV), provide valuable information on the impact of convection on the in-cylinder UHC and CO distributions. Hardware and vector processing details can be found in Colban et al. [21]. Note that clearance volume corrections for out-of-plane motion biases due to the swirl velocity were performed. These corrections were not performed within the bowl, however, since both the radial and axial velocity components are affected by out-of-plane motion.

SIMULATION METHODOLOGY

The details of both the homogeneous reactor and the multi-dimensional simulations have been described in detail by Ekoto et al. [12]; thus, only the key points are summarized here.

HOMOGENEOUS REACTOR SIMULATIONS – Homogeneous reactor simulations provide insight into the impact of pressure, temperature, dilution, and mixture stoichiometry on the expected yields of CO and UHC, albeit while neglecting mixing and heat transfer present in a realistic engine environment. The simulations were performed using CHEMKIN 4.1.1, employing the Lawrence Livermore National Laboratory detailed n-heptane mechanism [29], augmented with GRI-Mech 3.0 NO_x chemistry [30]. Pressure was constrained to match the experimental pressure trace, while the energy equation—including pressure boundary work—was employed to solve for temperature. The computations, performed for initial ϕ ranging between 0.05 and 2.0, commenced after a 9°CA ‘mixing delay’ from the start-of-injection. The initial mixture temperature for each ϕ was set to the temperature achieved when coolant temperature liquid fuel (360 K) vaporized and adiabatically mixed with the hotter ambient charge (~920 K).

MULTIDIMENSIONAL SIMULATIONS – Multi-dimensional simulation results were generated using the KIVA-3V CFD code [31] coupled with the CHEMKIN chemistry solver. Computational efficiency was improved by employing a 1/7th-sector combustion chamber mesh consisting of 35,000 cells at inlet valve cutouts. Piston-top valve-cutouts were not represented. Further