

Sources of UHC Emissions from a Light-Duty Diesel Engine Operating in a Partially Premixed Combustion Regime

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ABSTRACT

Sources of unburned hydrocarbon (UHC) emissions are examined for a highly dilute (10% oxygen concentration), moderately boosted (1.5 bar), low load (3.0 bar IMEP) operating condition in a single-cylinder, light-duty, optically accessible diesel engine undergoing partially-premixed low-temperature combustion (LTC). The evolution of the in-cylinder spatial distribution of UHC is observed throughout the combustion event through measurement of liquid fuel distributions via elastic light scattering, vapor and liquid fuel distributions via laser-induced fluorescence, and velocity fields via particle image velocimetry (PIV). The measurements are complemented by and contrasted with the predictions of multi-dimensional simulations employing a realistic, though reduced, chemical mechanism to describe the combustion process. Homogeneous reactor simulations also employed to clarify the influence of chemistry (vs. mixing) on UHC oxidation, and to compare the behavior of the reduced chemical mechanism with a more detailed mechanism. The impact of injection timing on the UHC distributions is also examined.

At the completion of heat-release, UHC is found in three regions: near the injector tip and cylinder centerline, the bowl and central clearance volume, and the squish-volume. The centerline UHC is composed of partially-reacted fuel that leaks from the injector late in the cycle and of discrete liquid droplets, embedded within diffuse UHC associated with overly lean mixture. Within the bowl and central clearance volume, UHC stemming from both rich and lean mixtures is observed. With advanced

injection, UHC from lean mixtures dominate; with retarded injection rich-mixtures are dominant. In the squish-volume, UHC originating from piston-top films and ring-land crevice flows is observed with advanced and MBT injection timing, while with retarded timing, UHC from lean mixtures is dominant.

INTRODUCTION

With tightening worldwide supplies of crude oil and growing emphasis on reducing greenhouse-gas emissions, the roughly 30% increase in fuel economy—and corresponding decrease in CO₂ emissions—make compression-ignition (diesel) engines attractive relative to conventional spark-ignition engines. Conventional diesel combustion, however, leads to soot and nitrous oxide (NO_x) emissions that exceed regulated levels. Consequently, diesel particulate filters and NO_x aftertreatment devices are required, which adversely impact vehicle costs and can reduce fuel efficiency.

To minimize cost and efficiency penalties, low-temperature combustion (LTC) techniques are being actively investigated. Through a combination of enhanced fuel-air premixing and low peak combustion temperatures, LTC enables significant reductions of both soot and NO_x emissions, but a fuel efficiency penalty and increases in unburned hydrocarbon (UHC) and carbon monoxide (CO) emissions are often incurred. Understanding and minimizing the sources of these emissions, and the associated efficiency loss, is required if LTC techniques are to be advantageously employed.

In this work, we focus on one variant of LTC, partially-premixed compression ignition (PPCI). With PPCI combustion, a modest compression ratio (≈ 16) and very high levels of EGR produce an extended ignition delay, which allows for injection timing as early as $\approx -30^\circ\text{CA}^\dagger$ while maintaining appropriate heat-release phasing. These combustion systems, which have been studied under a variety of names (e.g. [1-6]), invariably exhibit increasing CO and UHC emissions as the dilution (EGR) rate is increased.

Sources of UHC and CO emissions include overly lean regions that burn slowly and are easily quenched by gas expansion and overly rich regions with insufficient O_2 to complete combustion [7, 8]. Additional emission sources can include wall and crevice quench layers as well as nozzle dribble [9-11]. Changes in engine operating conditions, geometry, or fuel injector will change the relative contributions from each of these sources. Occasionally, misfire is also cited as a possible source of elevated UHC and CO emissions. Recent cycle-resolved UHC measurements made under LTC-PPCI conditions have shown, however, that the coefficient of variation (COV) of UHC emissions remains relatively constant even as the mean emissions deteriorate [12]. Consequently, misfire—as well as cycle-to-cycle variations in the combustion process—are not thought to be dominant emission sources.

At moderate load (3–6 bar IMEP) and speed (1500–2000 rpm), several studies of PPCI combustion have concluded that CO emissions are dominantly formed in overly rich regions [5, 6, 13]. Evidence supporting this conclusion includes: a negative correlation between CO emissions and ignition delay, decreased CO emissions with increased injection pressure, a generally small impact of intake temperature on CO emissions, and the results of multi-dimensional simulations. Because UHC emissions generally track CO emissions, this conclusion suggests that UHC emissions may similarly have a significant component associated with rich-mixtures. In contrast, work at lighter load [14] has shown that a significant reduction in both UHC (and CO) emissions is achieved with increased charge temperature—behavior that is indicative of overly lean, chemical-kinetic-rate-limited emission sources. Evidently, there is no single source of UHC emissions that dominates over all operating conditions.

Identification of the various sources contributing to UHC emissions, and knowledge of how these sources change with operating conditions, is essential if effective strategies are to be devised to control them. Accordingly, the objective of this paper is to identify the in-cylinder sources of UHC in PPCI combustion systems, and to examine the impact of injection timing on these sources. This is accomplished through a combination of both experiments and numerical simulation. Experimental data considered include direct

[†] Crank angles given in this paper are relative to top dead center (TDC) compression

in-cylinder visualization of the spatial distribution of UHC using laser-induced fluorescence (LIF), visualization of liquid fuel through elastically scattered light, and measured flow fields acquired via particle image velocimetry (PIV). The simulation results include both homogeneous reactor simulations (simplified mixing but detailed chemistry) and multi-dimensional simulations (detailed mixing with simplified chemistry) which complement the experimental data.

ENGINE

All measurements were acquired in a single-cylinder direct-injection (DI) optically-accessible research engine based on a 4-cylinder General Motors 1.9L light-duty design. The head is outfitted with 4 valves angled $\approx 2^\circ$ from vertical and a central, vertical Bosch CRIP 2.2 injector. Bore geometry, valve timing and fuel injection characteristics are summarized in Table 1.

Reentrant bowl geometry, typical of a production engine, was preserved in the fused-silica piston top. A geometrically accurate representation of the piston bowl, which has a maximum internal radius of 25.1 mm, a bowl rim radius of 22.6 mm, and a maximum depth of 14.8 mm is shown in Figs. 3 and 4. The major geometric differences between a conventional piston design and the optical piston design are the optical piston's lower ring-pack position (resulting in 3–4 times the volume of a typical top ring-land crevice) and the absence of valve cutouts. Both of these features could impact UHC and

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	3.0 [bar]
SOI _{command}	-31.1,- 26.6 ,-15.8 [°CA]
SOI	-27.6,- 23.1 ,-12.3 [°CA]
EOI _{command}	-25.9,- 21.4 ,-10.6 [°CA]
EOI	-21.2,- 16.7 ,-5.9 [°CA]
[O ₂]	10 [%]
Engine Speed	1500 [rpm]
T _{intake}	90 [°C]
P _{intake}	1.5 [bar]
CR (Geometric / Effective)	16.7 / 14.0
Swirl Ratio:	2.2
Injector Characteristics: Bosch Common Rail CRIP2.2	
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

CO emissions stemming from the crevice and squish regions. Note that while the geometric compression ratio is 16.7, an effective compression ratio of 14.0 more closely matches cylinder pressures and combustion behavior predicted by a one-dimensional engine simulation model due to heat transfer effects associated with the increased crevice volume [15]. The upper liner had four, standard-grade fused-silica windows for admitting the laser sheet and viewing fluorescence. These windows, and the fused-silica piston top, likely produce combustion chamber surface temperatures that differ from conventional engines, which may impact both fuel film vaporization and oxidation processes near the walls. Despite these differences, the UHC and CO emissions behavior of a conventional single-cylinder test engine has been well-captured by this optical engine [16].

Cylinder pressure data were collected using a Kistler 6125B quartz pressure transducer mounted in the glow plug position and used to obtain indicated mean effective pressure (IMEP), apparent heat-release rate (AHRR), and ignition delay. The heat-release analysis was performed following an iterative, two-zone procedure using temperature and mixture dependent gas properties, as described by Kook et al. [6].

OPERATING CONDITIONS

Engine performance and emissions of soot, NO_x , UHC and CO were previously mapped for a wide range of intake O_2 concentrations ($[\text{O}_2]$), injection timings, and intake pressures [15]. UHC and CO emissions are most problematic at lighter loads, and thus a 3.0 bar IMEP baseline condition was selected. The start-of-injection (SOI) was selected to obtain the maximum indicated work for a fixed fueling rate. At the selected baseline $[\text{O}_2]$ of 10%, and a 1.5 bar intake pressure, adequate combustion efficiency ($\sim 98\%$) was obtained despite elevated UHC and CO emissions relative to higher $[\text{O}_2]$ —as shown in Fig. 1. By plotting UHC and CO emissions as their normalized heating value, CO emissions can be seen to dominate the efficiency loss.

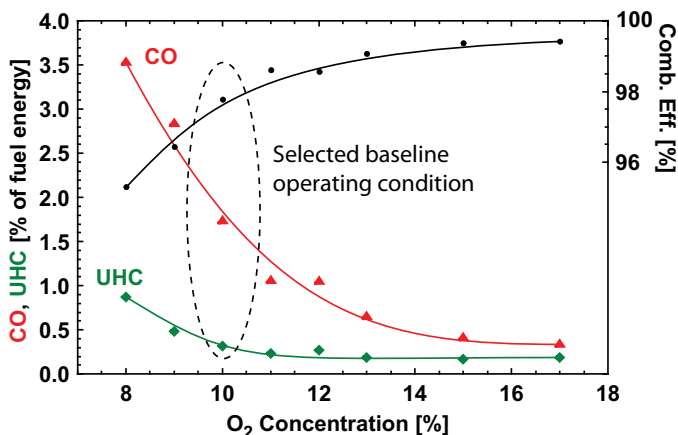


Figure 1 Emissions and combustion efficiency as dilution is increased at MBT timing.

The impact of advancing and retarding injection was also investigated. Relative to the baseline operating condition, the injection duration was held fixed, while the start-of-injection was either retarded or advanced such that the load decreased by roughly 15%. The different injection timings are summarized in Table 1.

To limit combustion chamber surface temperatures and prolong the lifespan of the optical pistons, skip-fired operation was employed wherein the engine was fired every fifth cycle. To maintain a consistent engine thermal state between tests, a strict 8 minute operating schedule was followed. The schedule began with 70 seconds of motored engine operation, to stabilize intake plenum pressures and preheat combustion chamber surfaces before starting skip-fired operation. A 20-second delay between the start of skip-firing and the start of measurement acquisition was employed to preheat the combustion chamber surfaces. A detailed discussion of the data acquisition procedure is presented in the experiments section. Finally, the engine was stopped and allowed to cool for the remainder of the schedule duration before starting the next run. During this time, accumulated soot and fuel film residue were cleaned from the quartz piston and liner windows.

Because the engine was skip-fired, simulated EGR was used to obtain the desired intake O_2 concentration, by diluting the intake charge with N_2 and CO_2 , in proportions that matched the specific heat ratio (at 600 K) of complete combustion products, while maintaining a constant intake mass flow rate of 8.9 g/s. The mass fraction of each species in the intake charge and the stoichiometric charge-fuel mass ratio that corresponds to the intake charge composition is provided in Table 2. The pressure traces and apparent heat-release rates for each condition are displayed in Fig. 2.

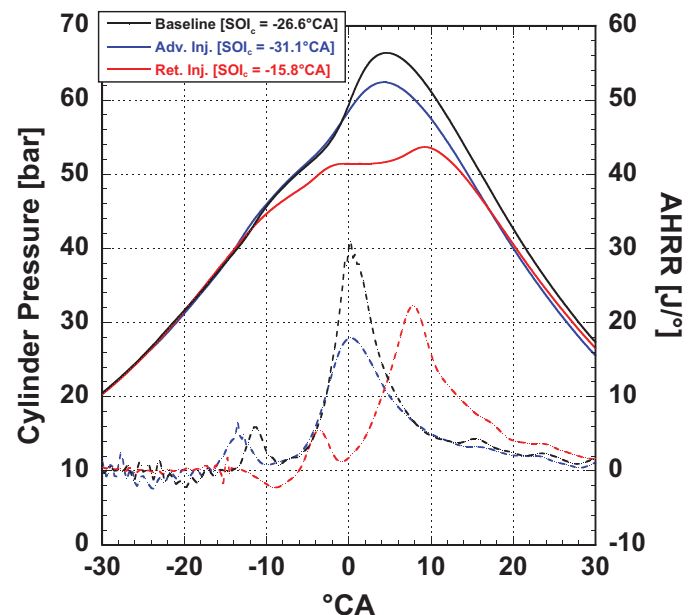


Figure 2 Characteristic cylinder pressure and heat-release traces for all conditions.

Table 2 Summary of intake charge mass fraction and stoichiometric charge-fuel mass ratio.

[O ₂]	Air	N ₂	CO ₂	Charge/Fuel Mass ratio
10%	0.460	0.402	0.138	32.45

EXPERIMENTS

UHC LASER INDUCED FLUORESCENCE (LIF) – Laser-induced fluorescence from CH₂O (formaldehyde), poly-aromatic hydrocarbons (PAH), and parent fuel compounds was excited using an 8 ns laser pulse from the third harmonic (355 nm) of a Nd-YAG laser (Spectra-Physics Pro-290). The laser beam was shaped into a 30 mm high, 500 μ m thick sheet by a concave/convex spherical lens pair with an effective focal length of 1800 mm, coupled with a -75 mm focal length cylindrical lens. The estimated sheet thickness variation was roughly ± 25 μ m throughout the cylinder. The vertical laser sheet entered the cylinder through the fused-silica windows in the upper cylinder liner, aligned with the axis of one of the 7 fuel jets (Fig. 3). For future reference, the “jet-axis plane” is defined as the plane on the right-hand side of the images, where a fuel spray is aligned with the incoming laser sheet. The “off-axis plane” refers to the plane on the opposite side of the combustion chamber (left-hand side), where the laser sheet bisects the angle between two fuel sprays. Because the laser fired at a rate of 10 Hz, but data were acquired at a rate of ≈ 3 Hz (on fired engine cycles), a laser shutter was used to prevent excessive laser strikes on the windows and optical piston. The laser pulse energy, typically 35 mJ, was monitored with a pyroelectric detector (Coherent J4-09).

It should be noted that in regions with only moderately rich pre-combustion equivalence ratios ($1 < \phi < 2$), homogeneous reactor simulations show that significant PAH formation is not expected [17]. However, even with the high dilution levels typical of PPCI combustion, CH₂O is completely consumed during the high-temperature combustion process for $\phi > 0.3$. Fluorescing compounds in the parent fuel are also likely to be destroyed early in the combustion process. Hence, the present PLIF diagnostic may be unable to image a potentially significant fraction of bulk-gas UHC embedded in the products of moderately rich combustion. Nevertheless, the PLIF diagnostic is useful for detecting UHC originating from overly-rich regions where PAH formation occurs, low-temperature (typically lean) regions where CH₂O is present, and regions where the parent fuel molecules have not yet been broken down.

Fluorescence emissions were collected in two distinct experimental configurations, also illustrated in Fig. 3. One supplied planar (two-dimensional) spatial information, and the other provided spectral information along the jet-axis side of the cylinder.

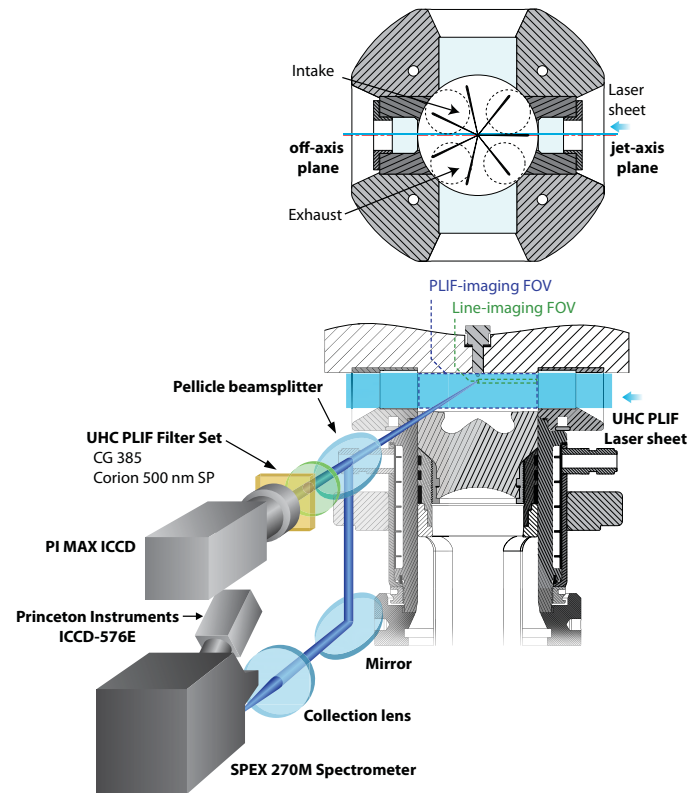


Figure 3 Cross-section of the optical engine and schematic representation of the experimental set-ups for 2-D PLIF and 1-D spectrally-resolved LIF imaging of UHC.

Planar (PLIF) Imaging – PLIF images were obtained using a Roper Scientific PI-Max intensified camera with a resolution of 512 x 512 pixels, fitted with a Nikkor 50 mm glass lens and a +4 diopter close-up lens. A 100 ns camera gate was employed. The spectral range of the fluorescent emissions imaged was limited to approximately 385–500 nm using the filter set indicated in Fig. 3, which encompasses most of the emissions from the $A^1A_2 \rightarrow X^1A_1$ CH₂O transition [18]. To obtain the best focus while imaging through the curved bowl walls, an aperture setting of $f/16$ was employed.

For each test condition, 50 single-cycle PLIF images were acquired. To eliminate spurious signal from the windows and injector tip, a background correction was used. While the engine was motoring, the background image set was acquired. During post-processing, the average background image was subtracted from each fired image.

Large laser sheet irradiance variations, generated by refraction and reflections from the piston surfaces, were compensated for by performing a flat-field correction. For this purpose, motored-engine reference images were obtained at each crank-angle by seeding the intake charge with 3000 ppm CH₂O, generated by metering and vaporizing a 10% Fischer-Scientific formalin solution (3.7% [CH₂O]). A spatially-uniform mixture was ensured by mixing the CH₂O vapor with the main intake charge well upstream of the intake port. PLIF images acquired

during normal, fired operation were normalized by the flat-field images during image processing.

The laser sheet was partially blocked by the bowl lip and injector tip. Hence, PLIF imaging in the off-axis plane was restricted in the lower piston bowl and in the upper 2 mm of the clearance volume. In spite of the high $f/\#$ used, signal-to-noise levels during the flat-field correction were between 1.6 (in the bowl) and 2.5 (in the squish); sufficient for the desired qualitative spatial distributions.

Strong optical distortion from the curved combustion-chamber surfaces necessitated a distortion correction for images obtained both within the clearance and the bowl volumes. Separate, piecewise-linear distortion corrections [19] were derived for both volumes from images of an illuminated calibration grid, and used to reconstruct undistorted images. Since clearance volume distortion is due solely to the upper liner windows, it is not dependent on piston position and only a single distortion correction suffices for all crank angles. Within the bowl, a unique correction is required for each crank angle. Distortion-corrected clearance volume and bowl images were then recombined at the interface (the piston crown). Noise was reduced by using a 3×3 pixel median filter and the images were lightly smoothed by a 5×5 Gaussian filter ($2\sigma = 1.6$ pixels, corresponding to ~ 0.1 mm).

Spectrally-Resolved, One-Dimensional Imaging – One-dimensional, spectrally-resolved LIF images were acquired using a Spex 270M imaging spectrograph, equipped with a Princeton Instruments ICCD-576E intensified camera, as shown in Fig. 3. The setup is described in greater detail by Kim et al. [20]. To maintain sufficient signal strength, only half of the cylinder bore was imaged. Mean images, corresponding to 50 engine cycles, were integrated on-chip, employing the maximum intensifier gain. Due to severe optical distortion within the bowl, spectrally-resolved imaging was performed mainly in the clearance volume. The horizontal entrance slit of the spectrograph was set to a height of 0.5 mm, providing a 5.3 nm spectral resolution. Fluorescent emissions were collected from a 2.4 mm high segment of the laser sheet centered 3.0 mm below the piston head and spanning from the cylinder centerline to the bore wall. The measurement volume was positioned high in the cylinder to enable spectral characterization of fluorescence from the clearance volume beginning at 25°CA —the start of the late-cycle burnout period.

A background correction, like that applied to the PLIF images described above, was employed to minimize interferences, which were most pronounced near the injector tip. Likewise, noise was removed with a 3×3 pixel median filter and a 13×13 Gaussian smoothing filter ($2\sigma = 4.8$ pixels, corresponding to ~ 0.5 mm and ~ 1 nm in the spatial and spectral axes respectively). A calibration target image was used to define 3 spatial

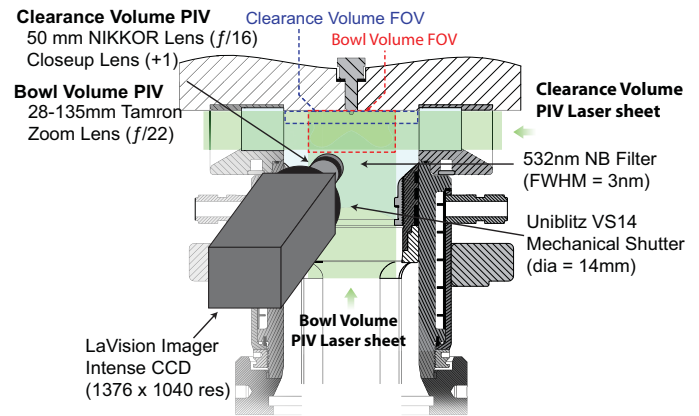


Figure 4 Experimental setup for PIV and elastic light scatter measurements within the clearance and bowl volume.

regions within the clearance volume: the centerline, the bowl and central clearance volume, and the squish-volume. For each wavelength, the pixels within each region were summed to obtain a spectrum characteristic of the LIF emissions. Integrated spectra from each bin were band-pass filtered to isolate distinct spectral peaks. Similar to the method employed by both Lachaux and Musculus [21], and Genzale et al. [8], the correlation coefficient (R_{xy}) was calculated between band-pass filtered fired-cycle and reference CH_2O spectra, to quantify their similarity. A cutoff value of $R_{xy} > 0.6$ serves as a reasonable indication of CH_2O fluorescence.

ELASTIC LIGHT-SCATTERING AND PIV – Mean velocity fields provide valuable information on the impact of convection on the in-cylinder UHC distributions. For the present study, the velocity fields were measured using particle image velocimetry (PIV). Details of the hardware setup, image correction, and velocity vector processing are provided by Colban et al. [19], while a schematic is given in Fig. 4. Measurements of elastic light scatter, indicative of the presence of liquid fuel, were also collected using the same experimental configuration.

An important detail concerning velocity vector post-processing is the impact of out-of-plane motion due to the swirl velocity. Out-of-plane motion biases velocity measurements at large radii due to the large viewing angles caused by the curved combustion chamber surfaces and the resulting projection of the swirl velocity onto the image plane. The impact of out-of-plane motion is corrected for within the clearance volume, where only the radial component is affected, by assuming the flow is axisymmetric. While this assumption is unlikely to be strictly valid, particularly at crank angles near the injection and rapid combustion event, we believe the corrected flow fields are a better representation of reality than the uncorrected flow fields. Within the bowl, both the radial and axial velocity components are affected by out-of-plane motion. Thus, no correction was made in this region.

SIMULATION METHODOLOGY

HOMOGENEOUS REACTOR SIMULATIONS – Homogeneous reactor simulations can provide insight into the impact of pressure, temperature, dilution, and mixture stoichiometry on the expected yields of CO and UHC, even though they neglect mixing and heat transfer present in a realistic engine environment. Simulations were performed using CHEMKIN 4.1.1, employing the Lawrence Livermore National Laboratory detailed *n*-heptane mechanism [22], augmented with GRI-Mech 3.0 NO_x chemistry [23].

For the reactor simulations, the pressure was constrained to match the experimental pressure trace, and the adiabatic temperature was determined from the energy equation. Computations were initialized at SOI plus a ‘mixing delay’ of 9°CA. The initial mixture temperature varied with equivalence ratio ϕ and was set to the temperature achieved when liquid fuel, initially at 293 K, is mixed adiabatically with the core gases at an estimated temperature of 830 K. These simulations improve on the earlier work of Kim et al. [20] by assuming an initial core charge temperature more appropriate to the low compression ratios of LTC combustion, allowing for the impact of dilution on the initial temperature due to the lower specific heat ratio of exhaust gases, and extending the calculations over a broader range of initial equivalence ratios.

MULTIDIMENSIONAL SIMULATIONS – The multi-dimensional computational fluid dynamics (CFD) code used is a version of the KIVA-3V code [24] with improvements in various spray and chemistry models [25] developed at the University of Wisconsin-Madison Engine Research Center.

To improve computational efficiency, a sector mesh encompassing 1/7th of the combustion chamber was used, as shown in Fig. 5. Results are presented primarily from the jet-axis plane. However, the off-axis plane results are presented where appropriate. To adequately match the experimentally measured pressure traces without significantly altering the squish region geometry, additional volume was added to the top ring-land crevice by increasing its width to 0.5 mm, while keeping crevice depth identical to the experiment. The 1.588 mm piston-pin offset in the experiment was preserved in the model.

To achieve manageable computational times, the combustion process was modeled by the University of Wisconsin (Madison) Engine Research Center Primary Reference Fuel (ERC-PRF) reduced *n*-heptane chemical mechanism, characterized by 39 chemical species and 131 reactions [26]. The KIVA code provides CHEMKIN with the species and thermodynamic information in each computational cell and CHEMKIN returns new species information and energy release after solving for the chemistry. This reduced mechanism coupled with the CHEMKIN solver has been successfully applied in diesel

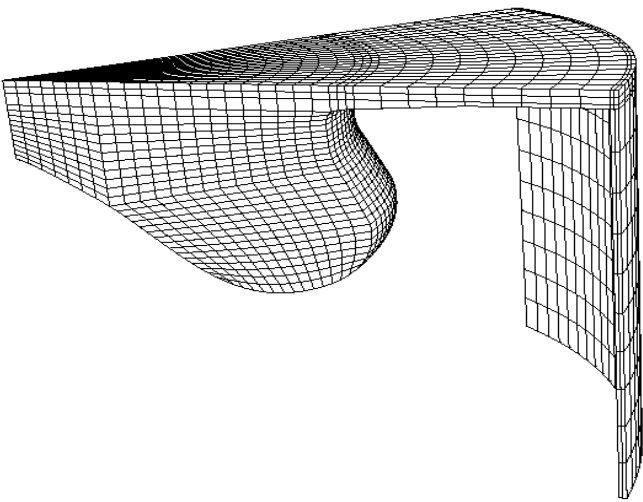


Figure 5 Computational sector mesh of one-seventh of the cylinder at TDC.

engine multidimensional simulations, and exhibits good agreement with experimental results [26, 27].

Relative to *n*-heptane, the physical properties of tetradecane more closely match diesel fuel (e.g., boiling point and density). Hence, these properties were used to calculate droplet breakup, collision/coalescence and evaporation. Conversions between *n*-heptane and tetradecane required for the chemistry computation were performed based on mass conservation, as appropriate.

Grid-size dependency can significantly impact simulation results [27, 28]. To minimize the dependency, updated spray models such as the gas-jet model [28, 29], the radius-of-influence (ROI) collision/coalescence model [30] and the mean collision time model [30] were used. Previous studies have shown that the updated spray models produce more reliable results that are relatively insensitive to grid-size in both engine simulations [28] and spray simulations of a constant volume combustion chamber [27]. The updated spray models were implemented into the KIVA-3V release 2 code, which

Table 3 Sub-models employed for the multi-dimensional simulations.

Ignition/combustion model	Chemkin chemistry solver
Chemkin mechanism	ERC-PRF <i>n</i> -heptane mechanism
NO _x mechanism	Reduced GRI mechanism
Soot model	2-step phenomenological model
Atomization/breakup model	KH-RT model
Liquid/Gas phase momentum coupling	Gas-jet model
Collision model	Radius-of-influence collision model
Time-step calculation	Mean collision time step model

includes the Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) spray atomization and breakup model [31] and the renormalization group (RNG) κ - ϵ turbulence model [32]. The detailed sub-models are listed in Table 3.

RESULTS

HOMOGENEOUS REACTOR SIMULATIONS – It is well established that increasing charge dilution slows chemical reaction rates, mainly through a reduction in combustion temperature resulting from the increased ambient specific heat. Consequently, for lean mixtures, increasing dilution requires an increase in the equivalence ratio in order to reach critical oxidation temperatures—below which UHC and CO oxidation is excessively slow. For UHC and CO the critical temperatures are approximately 1200 and 1500 K, respectively [20].

The impact of dilution on rich-mixtures is not well understood, however. Although rich-mixture UHC and CO oxidation is generally limited by the available O_2 (rather than temperature), substantially complete oxidation of UHC-to-CO is possible even in moderately rich environments. To clarify the impact of dilution on rich-mixture oxidation, homogeneous reactor simulations were performed up to equivalence ratios of 2.

Figure 6 compares the oxidation behavior of the full and reduced chemical mechanisms. The red and orange shaded regions indicate the crank angle range for each initial equivalence ratio where the temperature exceeds

the respective critical CO and UHC oxidation temperatures. Also shown in Fig. 6 are isopleths representing the CO or UHC yields corresponding to 2% of the fuel energy embodied in either UHC (20 g/kg-fuel) or CO (88 g/kg-fuel). The regions within the isopleths represent equivalence ratios giving acceptable UHC or CO emissions from an efficiency standpoint.

Several observations can be made from Fig. 6:

- The full mechanism results show that for moderately lean and rich mixtures ($0.5 < \phi < 1.4$), once the cycle temperature has reached 1200 K, oxidation occurs rapidly (within 5°CA). A similar correlation, albeit within a smaller equivalence ratio band, is observed between the CO isopleth and cycle temperatures above 1500 K. The required temperature for acceptable CO oxidation agrees well with the 1500 K limit previously found with no dilution [33]. Dilution thus has relatively little impact on the kinetics of oxidation, other than its role in reducing combustion temperatures.
- A comparison of the full mechanism, lean-region isopleths for UHC and CO indicates acceptable oxidation of UHC is achieved at leaner equivalence ratios (and lower peak temperatures) than needed for acceptable CO oxidation. This is caused by the relatively slow rates governing the final CO-to- CO_2 oxidation step. Consequently, the formation of overly lean regions will likely impact CO emissions more than UHC emissions. The exception occurs at very lean equivalence ratios, when little oxidation occurs and little CO is formed. Generally, however, steps taken to reduce lean region emissions (e.g. increased intake temperature) will likely impact UHC emissions first and to a greater extent than CO emissions.
- Comparing the full mechanism rich-limit isopleths, acceptably low UHC levels are achieved at higher equivalence ratios ($\phi \approx 1.4$) than for CO ($\phi \approx 1.0$). This difference is due to the initial oxidation of UHC to CO, followed by the oxidation of CO to CO_2 if sufficient O_2 is present. Consequently, when UHC and CO emissions stem from overly rich regions (emissions are mixing-limited) it will generally be more difficult to reduce CO emissions than UHC.
- Comparison of the predicted equivalence ratio needed to bring the lean-limit CO yield below 88 g/kg-fuel (numerical values extracted from Fig. 6 are provided in Table 4), shows that the full mechanism requires a higher ($\phi_{CO} = 0.59$) equivalence ratio than the reduced mechanism ($\phi_{CO} = 0.50$). Hence, the reduced mechanism may result in lower predictions of CO from lean regions. Both mechanisms predict the rich equivalence ratio limit for adequate CO oxidation to be at stoichiometric conditions.

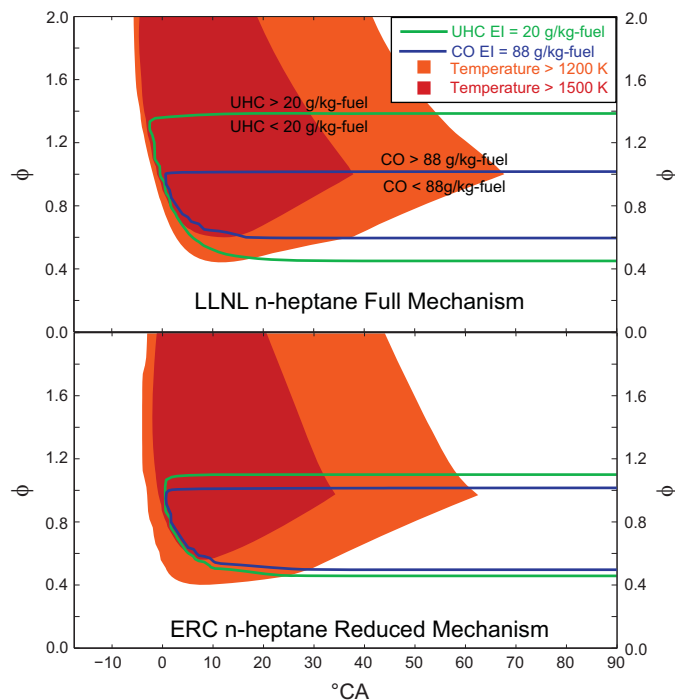


Figure 6 Isopleths corresponding to 2% of the fuel energy for UHC and CO, as a function of crank angle and equivalence ratio. Shaded regions identify where temperatures exceed 1200 and 1500K, for the UHC and CO plots, respectively.

Table 4 Lean and rich limit ϕ for CO and UHC, based upon pressure-constrained homogeneous reactor yield at 90°C. Lean and rich limits correspond to 2% of the fuel energy (UHC EI = 20 g/kg-fuel, and CO EI = 88 g/kg-fuel).

	Rich ϕ_{CO}	Rich ϕ_{UHC}	Lean ϕ_{CO}	Lean ϕ_{UHC}
LLNL Mech.	1.02	1.39	0.59	0.45
ERC-PRF Mech.	1.02	1.12	0.50	0.50

Table 5 Composition of the lean and rich limit homogeneous reactor UHC yield in g/kg-fuel at 90°C, where the UHC constitutes 2% of the fuel energy (20 g/kg-fuel).

Rich Limit UHC	ϕ	CH ₄	C ₂ H ₂	C ₂ H ₄	other
LLNL Mech.	1.39	8.5	10.6	0.9	0.0
ERC-PRF Mech.	1.12	19.6	0.3	0.0	0.1

Lean Limit UHC	ϕ	CH ₄	C ₂ H ₂	C ₂ H ₄	C ₃ H ₄	other
LLNL Mech.	0.45	14.2	0.9	4.4	0.0	0.5
ERC-PRF Mech.	0.50	17.7	0.0	0.0	2.0	0.3

- Comparing the lean-limit equivalence ratios for adequate UHC oxidation in Fig. 6 and Table 4, the full mechanism requires a lower equivalence ratio than the reduced mechanism. Consequently, the reduced mechanism will likely produce higher estimates of UHC stemming from lean regions than the full mechanism. The higher lean UHC emissions predicted by the reduced mechanism may be one reason for its lower CO predictions.
- For rich initial equivalence ratios, the limit predicted for adequate UHC oxidation by the reduced mechanism ($\phi_{UHC} = 1.12$) is significantly less than what is predicted by the full mechanism ($\phi_{UHC} = 1.39$), and the reduced mechanism might be expected to considerably over-predict UHC emissions stemming from moderately rich regions.
- From Table 5, the composition of rich-region UHC predicted by both mechanisms at the limiting equivalence ratio differs significantly. Methane (CH₄) dominates the rich-limit UHC yield when the reduced mechanism is used. In contrast, when the full mechanism is used, methane accounts for less than 1/2 of the UHC yield while significant contributions from acetylene (C₂H₂) and ethylene (C₂H₄) occur. Since acetylene is an important precursor to PAH formation, its yield may significantly impact predicted soot formation rates. At the lean limits, the two mechanisms exhibit better agreement in overall mixture composition, although the full mechanism predicts a small amount of acetylene and ethylene while the reduced mechanism instead predicts a small amount of cyclopropene (C₃H₄).

EXPERIMENTAL AND MULTIDIMENSIONAL SIMULATION RESULTS – In this section, the development of the UHC distribution is illustrated as the cycle progresses from injection through mixing, combustion, and expansion for each operating condition. Recall for the injection timing sweep that start of injection command (SOI_c), relative to the baseline condition (SOI_c=-26.6°C), is either advanced (SOI_c=-31.1°C) or retarded (SOI_c=-15.8°C) such that IMEP decreases roughly 15%.

The mixture fraction f , which characterizes the mixing between a fuel stream (stream 1) and an oxidizer stream (stream 2) is a useful parameter for examining the impact of in-cylinder mixing, and will be used in lieu of the equivalence ratio to examine multi-dimensional simulation results. Typically, the mixture fraction f is defined in terms of a conserved scalar Z as

$$f \equiv \frac{Z - Z_2}{Z_1 - Z_2} \quad (1)$$

Z is usually selected to be the mass fraction of the elements in the fuel stream. Because Z is conserved as combustion progresses, f characterizes the state of the mixing between streams 1 and 2, irrespective of the degree of reaction. The mixture fraction can be related back to a corresponding (pre-combustion) equivalence ratio through the following relation:

$$\phi = \frac{fr}{1-f} \quad (2)$$

where r is the stoichiometric charge-fuel mass ratio given in Table 2. With this r , the stoichiometric mixture fraction is approximately 0.03.

Injection and initial mixture preparation – The injection event determines the in-cylinder distribution of both liquid and vapor-phase fuel that results in UHC and CO emissions from liquid films, wall or crevice quench regions, and incomplete bulk-gas oxidation. Changes to injection timing directly impact mixture preparation by altering the ambient thermodynamic conditions (which influences fuel jet entrainment, penetration rate, and vaporization) and spray targeting (which influences the gross initial fuel distribution and in-cylinder flow structure).

Liquid penetration – The reduced compression ratio and early injection timing employed for PPCI combustion increases the liquid-phase fuel penetration over that of conventional diesel combustion due to lower ambient density during the injection event. Cooled intake charge and increased charge specific heat (due to high CO₂ and H₂O content) also contribute to lower ambient temperatures and delayed vaporization. Consequently, if the injector included angle is sufficiently large, liquid fuel can form films on the piston top, wet the cylinder walls, and enter the ring-land crevice.

