

Optical Diagnostics and Multi-Dimensional Modeling of Spray Targeting Effects in Late-Injection Low-Temperature Diesel Combustion

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ABSTRACT

The effects of spray targeting on mixing, combustion, and pollutant formation under a low-load, late-injection, low-temperature combustion (LTC) diesel operating condition are investigated by optical engine measurements and multi-dimensional modeling. Three common spray-targeting strategies are examined: conventional piston-bowl-wall targeting (152° included angle); narrow-angle floor targeting (124° included angle); and wide-angle piston-bowl-lip targeting (160° included angle). Planar laser-induced fluorescence diagnostics in a heavy-duty direct-injection optical diesel engine provide two-dimensional images of fuel-vapor, low-temperature ignition (H_2CO), high-temperature ignition (OH) and soot-formation species (PAH) to characterize the LTC combustion process. Multi-dimensional simulations, which agree well with the optical engine measurements, provide a three-dimensional picture of the fuel-air mixing processes and quantitative analysis of the soot, UHC and CO formation and oxidation.

The combined optical measurements and model simulations show that jet interactions with the piston bowl (jet-bowl) and with neighboring jets (jet-jet) can significantly influence pollutant formation and oxidation processes. With a conventional piston-bowl-wall targeting, the fuel jet impinges at the piston-bowl wall prior to ignition and merges with neighboring jets, where substantial fuel-rich soot-formation regions develop. The jet-bowl interaction also leads to a rebound of the jet-

head away from the piston bowl during late-cycle oxidation processes, enhancing the oxidation of soot, UHC and CO. By using a narrow-angle floor targeting, the fuel jet impinges at the piston-bowl floor and is redirected up along the bowl wall rather than towards neighboring jets, reducing jet-jet interactions. The suppression of these jet-jet interactions leads to less soot formation within the piston bowl. However, this altered jet trajectory eventually causes impingement at the cylinder head, creating a fuel-rich recirculation region where high levels of soot and CO form. By using a wide-angle piston-bowl-lip targeting, the jet is split between the piston bowl and squish region, which also reduces jet-jet interactions and soot formation within the bowl, but additional soot formation occurs in the squish region and total soot formation is not reduced. In addition, there is less rebound of the jet away from the piston-bowl wall and late-cycle oxidation of soot, UHC and CO is compromised.

INTRODUCTION

Low-temperature combustion (LTC) strategies are of increasing interest to diesel engine manufacturers because they can significantly suppress the formation of nitrogen oxide (NO_x) and soot during the combustion process, thus minimizing or potentially eliminating the need for costly aftertreatment devices. With these strategies, NO_x and soot suppression is typically achieved by charge dilution with exhaust gas recirculation (EGR) and fuel-air premixing prior to ignition. However, the accomplishment of pre-ignition

fuel-air premixing with conventional diesel fuels, which have low volatility and a high autoignition propensity, is not trivial. Accordingly, as LTC research has evolved, different strategies have been investigated to provide the required fuel-air premixing. These strategies typically fall into two major categories, defined by their fuel-injection timing relative to top-dead-center (TDC). One common strategy that naturally provides time for fuel-air premixing prior to ignition, uses an early staged injection well before TDC, allowing a relatively long premixing period prior to ignition (e.g. [1-3]). Alternatively, strategies using a later injection, near or just after TDC, have also been developed which feature a shorter premixing period (e.g., Nissan's "MK" concept [4,5]), but still demonstrate low NO_x and soot emissions commensurate with early-injection LTC strategies.

Challenges with the implementation of early-injection LTC have spurred a significant body of research aimed at optimizing fuel-injection geometries and injection timing for these strategies. With a low-density injection environment, early injections are susceptible to long liquid penetration lengths [6]. Accordingly, liquid wetting of in-cylinder surfaces, especially the cylinder liner, has been identified as a major drawback for early-injection LTC [1], contributing to increased UHC emissions and oil dilution. To address these issues, researchers have investigated many approaches, from complete redesign of the fuel injection geometry (e.g., IFP's narrow-angle NADI concept [2]) to careful studies of injection timing for optimized spray/bowl interaction [7,8,9]. From these and other studies, two different spray-targeting strategies dominate the literature as the most promising solutions for optimizing performance and emissions in early-injection LTC strategies. These include a narrow-angle injection, targeting the spray down towards the crown of the piston bowl (e.g., [2,8]) to avoid liquid wall impingement at the cylinder wall, and a wider-angle spray in combination with a slightly later injection timing (20° to 30° before TDC), targeting the piston-bowl lip (e.g., [7,9]) to direct the spray into the piston bowl. Though these targeting strategies arose primarily to address wall-wetting issues, researchers have also found that they can improve other mixing processes, enhancing pre-ignition mixing and soot, UHC and CO oxidation [9,10,11,12].

Late-injection LTC strategies, with injection timings near those of conventional diesel combustion strategies, have circumvented an immediate need for this type of injection system redesign. With injection near TDC, gas densities are higher, reducing or eliminating the problems with liquid impingement that can occur with early injections into a low-density environment [6]. Additionally, the injection is directed into the bowl when the piston is at TDC, eliminating the motivation to employ a narrow-angle spray to avoid cylinder-wall wetting. However, since early-injection LTC research has demonstrated that spray targeting can positively influence mixing and oxidation processes beyond the elimination of the wall-wetting problem, it is conceivable

that these spray-targeting strategies may offer benefits under late-injection LTC operating conditions too.

Indeed, as the understanding of these LTC combustion regimes has grown, it is unclear whether conventional injector geometries are optimal for fuel-air mixing and pollutant-emissions control. Optical measurements in engines and in diesel sprays studies have revealed that jet mixing, combustion and pollutant-formation processes occur differently in LTC than in conventional diesel combustion. Soot formation occurs primarily downstream in the head of the jet [13]. This is in contrast to the upstream soot-producing core found in conventional diffusion-flame diesel jets [14]. This shift is due to the charge dilution employed in LTC [15] and mixing between the end of injection and second-stage ignition. Rapid mixing after injection can produce leaner mixtures that do not form soot throughout much of the fuel jet, but over-leaning can also increase unburned hydrocarbons (UHC) [16] and carbon monoxide (CO) emissions [17].

Recently, our optical measurements in a heavy-duty direct-injection diesel engine have revealed that spray targeting does influence mixing and combustion processes under late-injection LTC operating conditions [18]. These processes appear largely affected by the jet-bowl interaction and ensuing jet-jet interactions that occur prior to ignition. Indeed, since soot formation typically occurs mainly at the head of LTC fuel jets, the interaction of this region with the piston-bowl surfaces and neighboring jets may be expected to affect the fate of the soot formation or oxidation processes. Additionally, the jet-bowl and jet-jet interactions appear to affect late-cycle bulk flows, which can influence LTC oxidation processes [9]. This may be especially relevant given the increased unburned hydrocarbon (UHC) and carbon-monoxide (CO) emissions that often arise under LTC regimes.

These optical measurements provide a qualitative picture of spray targeting effects under LTC conditions, but due to a lack of direct emissions measurements, they cannot provide a direct link to their effect on engine-out emissions. Furthermore, the measurements only accessed a limited portion of the combustion chamber, leaving open questions concerning the physical processes occurring outside of the probed regions. In the current work, we use a validated multidimensional model of the optical engine to perform a detailed evaluation of these previously published optical measurements [18]. We compare the model predictions against the optical measurements, stepping through each phase of the combustion process, from initial air-fuel mixing to first- and second-stage ignition and combustion, through late-cycle oxidation. Finally, we use the multidimensional model predictions to provide a quantitative interpretation of the experiments with a more conclusive evaluation of spray targeting strategies for late-injection LTC.

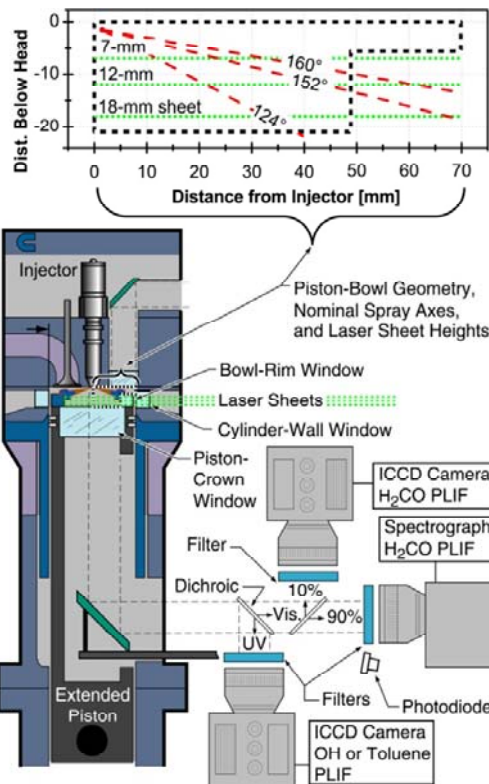


Figure 1: Schematic diagram of the optically-accessible direct-injection diesel engine and optical diagnostic setup (bottom). Illustration of nominal spray axes for injector nozzles studied relative to laser sheets and piston-bowl geometry with piston at TDC (top).

EXPERIMENTAL SET-UP

OPTICAL ENGINE AND OPERATING CONDITIONS - Experiments were performed in a single-cylinder optically-accessible version of a Cummins N-series heavy-duty direct-injection (DI), 4-stroke diesel engine. Figure 1 shows a schematic of the engine, and Table 1 summarizes the specifications of the engine. The engine has a bore of 140 mm and a stroke of 152 mm, yielding a displacement of 2.34 liters per cylinder. The intake-port geometry of the production cylinder head, which has a steady-state swirl ratio of 0.5 on a flow bench, is preserved in the optical engine. A complete description of the engine is available in Refs. [14,19,20].

As shown in Figure 1, the engine is equipped with an extended piston and flat piston-crown window to provide optical access through the bottom of the piston. Windows located around the top of the cylinder-wall provide cross-optical access for the laser-based imaging diagnostics. A window in the piston bowl-wall provides laser access into the piston bowl with the piston near TDC.

As specified in Table 1, the engine is equipped with a Cummins XPI, high-pressure, solenoid-actuated common-rail fuel injector. For the experiments presented here, the injector delivered fuel through an 8-hole,

Table 1: Engine, Injector and Fuel Specifications

Engine base type	Cummins N-14, DI diesel
Number of cylinders	1
Cycle	4-stroke
Number of intake valves	2
Number of exhaust valves	1*
Combustion chamber	Quiescent, direct injection
Swirl ratio	0.5
Bore	139.7 mm [5.50 in]
Stroke	152.4 mm [6.00 in]
Displacement	2.34 liters [142 in ³]
Squish Height	5.5 mm [0.22 in]
Connecting rod length	304.8 mm [12.00 in]
Piston pin offset	None
Geometric compression ratio	11.2:1
Simulated compression ratio	16:1
Combustion Chamber Geometry:	
Piston-bowl diameter	97.8 mm [3.85 in]
Piston-bowl depth	16.0 mm [0.63 in]
Injector Included Angle	124°, 152°, or 160°
Fuel Injector:	
Fuel Injector Type	Common-rail, solenoid actuated
Number of Holes & Arrangement	8, equally-spaced
Rail Pressure	1600 bar
Orifice Treatment	None (square-edged)
Nominal Orifice Diameter	0.196 mm
Orifice L/D	5
Base Fuel (by volume)	71% n-heptane, 29% iso-octane
Fuel Tracer (by volume)	1.0 % Toluene

* In this optically accessible diesel engine, one of the two exhaust valves of the production cylinder head was replaced by a window and periscope.

0.196 mm orifice, mini-sac injection cup. As shown in the schematic at the top of Figure 1, three different injector nozzle tips were implemented in this study to vary the spray targeting. With the piston at TDC (nominal injection time used in this study), this collection of nozzle tips allowed us to direct the fuel sprays toward the piston bowl-floor, the vertical center of the bowl-wall (conventional targeting for this engine), and the top of the bowl-wall, using spray patterns with included angles of 124°, 152° and 160°, respectively. These spray angles are referred to as the narrow-angle (124°), baseline (152°) and wide-angle (160°) sprays throughout the text and are representative of the narrow-angle [2], conventional diesel [14] and bowl-lip targeted sprays [9] that have been widely investigated in the literature under early-injection LTC operating conditions.

The engine was operated at a late-injection LTC operating condition, with a single fuel injection event starting at 0° after TDC (ATDC). This operating

Table 2: Engine operating conditions.

	Combusting	Non-Combusting
Engine Speed, RPM	1200	
Nominal GIMEP, kPa	400	-
Quantity of injected fuel, mg	56	
Injection duration, ms (CAD)	0.94 (6.75)	
Actual SOI, °ATDC	0	
Intake oxygen, % (by volume)	12.7	0
Equivalent EGR rate, %	60	-
Global equivalence ratio	0.27	-
Estimated motored TDC density, kg/m ³	22.2	22.2
Estimated motored TDC temp., K	838	838
Intake temperature, °C	70	72
Intake pressure, kPa abs.	202	206
BDC temperature, °C	78	79
16:1 BDC temperature, °C	49	49
16:1 BDC pressure, kPa abs	129	129

condition was selected using the characteristics of other reported late-injection LTC research as a guide (e.g. [4,5]) and has been previously demonstrated to perform with very low NO_x and soot emissions in this engine with diesel fuel [13]. The fuel injection duration was approximately 0.94 ms, or 6.75 crank angle degrees (CAD) at 1200 RPM, and the fuel rail pressure was 160 MPa (see Table 2). This injection delivered approximately 56 mg of fuel and yielded a nominal gross indicated mean effective pressure (GIMEP) of 400 kPa. This low-load condition was chosen to avoid damaging the large piston-crown window by limiting the maximum energy release during combustion. In addition, to minimize thermal loading on the optical engine, the injector was fired one out of ten cycles and an electric dynamometer maintained constant engine speed. To simulate EGR, the intake air stream was diluted with nitrogen to an oxygen concentration of 12.7% oxygen (by volume). Note that the intake temperature and pressure are higher than typical for production engines because of the low compression ratio of the optical engine. Due to compromises necessary to implement optical access in the engine, the geometric compression ratio is about 11.2:1, compared to 16:1 in the production version of this engine. As a result, elevated intake-air temperatures and pressures are required to yield charge conditions at TDC typical of a production engine.

Quantitative fuel-vapor concentration measurements, performed in the optical engine with a fuel-tracer fluorescence diagnostic, required that the engine be supplied with an oxygen-free (non-combusting) 100% N₂ intake stream for a portion of the experiments. This environment avoided oxygen quenching of the

fluorescence and ensured that the fuel tracer (toluene) would not break down during combustion. Both of these effects can significantly confound quantitative interpretation of fuel-tracer measurements [21]. The non-combusting condition presented in Table 2 features a different intake temperature and pressure from the combusting condition to replicate the estimated in-cylinder TDC density and temperature of the combusting condition, accounting for the lower specific heat ratio of the pure nitrogen intake stream. By matching the ambient density and temperature, the fuel jets should penetrate and mix with the charge gases at a similar rate under the combusting and non-combusting conditions [22].

The fuel for both the combusting and non-combusting experiments was a gasoline primary reference fuel (PRF) blend of 71% (by volume) HPLC-grade n-heptane (C₇H₁₆) and 29% (by volume) HPLC-grade iso-octane (C₈H₁₈), or PRF29, to which 1% (by volume) toluene (C₇H₈) was added as a tracer for the direct measurement of fuel concentration. This blend of n-heptane and iso-octane well replicates the ignition and heat-release characteristics of a typical U.S. diesel fuel [23], while providing an optically clean fuel suitable for fluorescence measurements. Like most pure alkanes, n-heptane and iso-octane display very little fluorescence under UV excitation [21]. This is beneficial for the measurement of combustion species like OH and formaldehyde, which require excitation at UV wavelengths. Diesel fuel, on the other hand, contains many absorbing and fluorescing species, which can obscure these measurements [24]. This choice of fuel also provides boiling points that are lower than diesel fuel, ensuring a fully vaporized, well-mixed calibration condition for the fuel-tracer diagnostic [16].

This PRF fuel does differ in physical characteristics from a typical diesel fuel, which may be expected to influence certain processes. For example, the higher volatility of the PRF fuel compared to diesel fuel will decrease liquid penetration of the spray. Also, the fuel structure and components are not the same as diesel fuel and are likely to produce different pollutant emissions levels. Though the PRF fuel vaporizes more rapidly than diesel fuel, previous measurements [24] show that for the operating conditions of this study, even diesel fuel is completely vaporized by the time of the optical measurements. Since the liquid fuel is well vaporized prior to ignition and the ignition delays are comparable between the two fuels [23], the pre-ignition mixture distributions are expected to be similar. This investigation is intended to characterize the mixing, ignition, combustion, pollutant formation and oxidation processes of a LTC strategy and to assess the influence of spray-targeting on these combustion characteristics. While the absolute performance and emissions of these strategies may be somewhat different than for a real diesel engine with real diesel fuels, the resulting fundamental understanding of these LTC processes should still be applicable to practical diesel engines.

MEASUREMENTS AND DIAGNOSTICS - Mixing, ignition, combustion, and pollutant-formation processes were studied using three different planar laser-induced fluorescence (PLIF) diagnostics and a volume-integrated natural luminosity measurement. Under combusting conditions, planar laser-induced fluorescence of OH was imaged simultaneously with formaldehyde and PAH fluorescence. The formaldehyde and PAH fluorescence were recorded together with a single camera, and were discriminated from each other using a separate emission spectrograph. To study the mixture development of the fuel jets, the vapor-fuel concentration was quantitatively measured using toluene fuel-tracer fluorescence under non-combusting conditions. Finally, combustion luminosity was directed to a photodiode to provide a general temporal progression of the overall in-cylinder soot luminosity. Brief descriptions of the PLIF techniques follow and further details of this multiple diagnostic set-up may be found in Ref. [23].

OH Planar Laser-Induced Fluorescence (OH-PLIF) – OH fluorescence was excited near 284 nm at 17 mJ per pulse with the frequency-doubled output of an optical parametric oscillator (OPO), pumped by the 355-nm third-harmonic of a Nd:YAG laser. The UV camera in Fig. 1 imaged the resulting fluorescence emission. A set of three filters helped to isolate the OH fluorescence and reject elastic scatter: (i) a 16 nm wide unblocked bandpass filter (BPF) centered at 312 nm isolated the OH fluorescence, (ii) a 358-nm short-pass filter rejected fluorescence from other species and other interference, and (iii) a 2-mm thick WG 305 long-wave-pass colored-glass filter helped to remove elastically scattered laser-light.

Combined Formaldehyde and PAH Planar Laser-Induced Fluorescence (F/PAH-PLIF) - Formaldehyde fluorescence was excited by the 355-nm beam of a frequency-tripled Nd:YAG laser at 60 mJ per pulse. The resulting fluorescence was imaged by the visible-light camera in Figure 1, equipped with two filters: (i) a CG385 long-pass colored glass filter, and (ii) a 40-nm wide blocked BPF centered at 408 nm. These filters helped to isolate the formaldehyde fluorescence from other sources of interference, including elastic scattering of the laser light, fluorescence from other species, and laser-induced soot incandescence. Although the filters removed much of the interference, some interference remained within the spectral band of the formaldehyde fluorescence emission. Because of the temporal and spatial location of the interference (as shown in the results), the most likely source is fluorescence from PAH, and potentially some laser-induced incandescence from soot late in the cycle. Thus, the technique reveals both formaldehyde and PAH fluorescence.

Formaldehyde fluorescence is verified from a region along the jet axis by directing a portion of the fluorescence emission onto the entrance slit of an Oriel 1/8-meter spectrometer using a 105-mm f/2.5 glass lens, as shown in Figure 1. A CG375 long-pass colored glass

filter was placed in front of the lens to help reject strong elastic scatter from the laser. The fluorescence spectrum was imaged onto an intensified CCD array at the exit of the spectrometer, capturing emission from 380 nm to 450 nm. The similarity of the recorded spectral emission to a reference formaldehyde spectrum is then quantified by calculating a correlation coefficient between the sample and reference spectra [25]. The correlation coefficients calculated for discrete regions of fluorescence along the jet axis are displayed in a colorbar at the bottom of each experimental image. By evaluating each fluorescence image with this semi-quantitative measure of formaldehyde presence, the spatial and temporal locations of formaldehyde and PAH species can be directly identified in the PLIF images.

Toluene Fuel-Tracer Planar Laser-Induced Fluorescence (T-PLIF) - Quantitative fuel-vapor concentrations were measured by toluene-tracer fluorescence, excited by the 80 mJ per pulse 266-nm frequency-quadrupled output of a Nd:YAG laser. The resulting fluorescence was imaged by the UV-camera in Figure 1. Two spectral filters isolated the T-PLIF signal from laser elastic scatter and other interference: (i) a WG295 long-wave-pass filter and (ii) a 25-nm wide blocked BPF centered at 300-nm. Details on the calibration of the toluene-tracer fluorescence signal for quantitative fuel-vapor concentration measurements are included in Ref. [23].

The laser beams for the PLIF diagnostics were converted into thin (less than 1 mm thick) sheets using a combination of cylindrical and spherical lenses. For the simultaneous OH and formaldehyde/PAH fluorescence diagnostics, the 284-nm and 355-nm beams were combined and overlapped using dichroic mirrors. For the toluene-tracer fluorescence diagnostic, a single 266-nm beam was used, without any other beams. As depicted in Figure 1, the sheets entered the cylinder horizontally, parallel to the firedeck (i.e., the bottom surface of the cylinder head). The laser sheets passed through a window in the cylinder wall to illuminate one of the fuel-jets that was in-line with the cylinder-wall and piston bowl-rim windows. After being clipped by the window apertures, the sheet was about 35 mm wide inside the combustion chamber. As illustrated at the top of Figure 1, the laser sheets were passed through the combustion chamber at three different heights; 7 mm, 12 mm and 18 mm from the firedeck surface, respectively. These laser sheet heights were selected to provide imaging of the fuel jet throughout the depth of the piston bowl when the piston was near TDC.

Soot Luminosity - In addition to the imaging techniques, combustion luminosity was also directed to a large-area (1 cm²) photodiode, as shown in Figure 1. A neutral-density filter with an optical density of 3 (nominally 0.1% transmission) attenuated the light reaching the photodiode so that it would not saturate. For conventional diesel combustion, soot luminosity is typically orders of magnitude brighter than chemiluminescence [26,27]. At LDC conditions, soot

and soot luminosity are much lower, but they are still much stronger than chemiluminescence. Furthermore, there was no detectable interference in the signals during the time of ignition, when chemiluminescence emission is expected to be strongest. Thus, the signal from the filtered photodiode represents primarily soot luminosity (non-sooting combustion yields essentially zero signal). The photodiode collected light from the entire combustion bowl, and its signal therefore represents a time-record of the overall combustion luminosity. Note that the field of view through the bottom of the piston bowl limits the collection of light to the combustion bowl and areas directly above. Accordingly, the photodiode signal is not representative of combustion processes outside of this field of view (i.e. in the squish and crevice volumes).

COMPUTATIONAL MODELING

CFD CODE - A modified version of the KIVA-3V, release-2 code [28] simulated the closed-valve portion of the engine cycle. Several improved submodels included a modified re-normalized group (RNG) $k-\varepsilon$ turbulence model [29] and a hybrid Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) model [30] to simulate spray atomization and break-up.

An integrated CHEMKIN chemistry routine [31] solved a surrogate diesel-fuel mechanism, based on n-heptane chemistry, with 30 species and 65 reactions. Although n-heptane chemistry is often used as a diesel surrogate in kinetic calculations, US Diesel fuels tend to have a lower cetane number (CN 40 - CN 46) than n-heptane (approx. CN 55) [32]. Hence, the reaction rates of the current mechanism are modified to predict the ignition delay of US Diesel fuel well [33]. This surrogate diesel-fuel mechanism is an appropriate choice to represent the n-heptane/iso-octane fuel-blend used in the experiments since the blend has an ignition delay similar to a US Diesel fuel. Furthermore, as shown later, the model-predicted cylinder pressure and heat-release rate exhibit good agreement with the experimental measurements under the LTC operating condition of this study.

The chemical kinetics were solved on the computational grid by treating each computational cell as a well-stirred reactor (sub-grid-scale turbulence-chemistry interactions are not considered). Previous computational studies have indicated that this approach is valid for LTC regimes, such as the condition investigated in the current work, where significant fuel-air premixing leads to a largely volumetric ignition process [34]. The non-chemical modeling of the liquid fuel (transport, break-up, evaporation, etc.) used the physical properties of n-heptane, which should closely match those of the n-heptane/iso-octane blend since iso-octane has similar physical properties as n-heptane.

NO_x chemistry was modeled using a reduced version of the Gas Research Institute (GRI) NO mechanism [35], adding 4 species (N, NO, NO₂ and N₂O) and 9 reactions

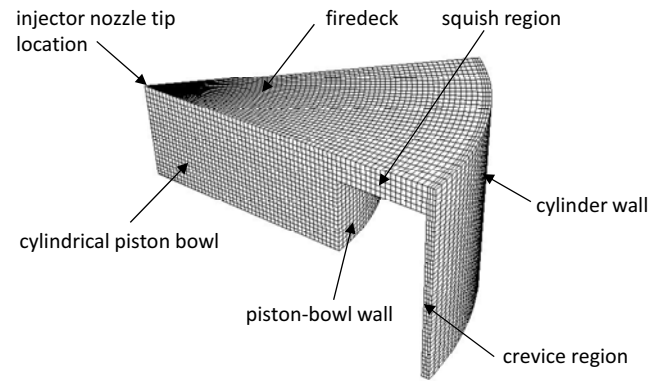


Figure 2: Computational mesh with piston at TDC. Mesh is composed of approximately 110,000 cells with the piston at BDC.

to the n-heptane mechanism. Three of the nine reactions are the extended Zeldovich reactions [36], and the other six account for thermal NO_x formation through NO₂ and N₂O reaction pathways. Soot emissions were predicted by the Hiroyasu soot-formation model [37] and the Nagle-Strickland-Constable (NSC) soot-oxidation model [38], using acetylene (C₂H₂) as the soot formation species.

COMPUTATIONAL MESH AND INITIAL CONDITIONS - The computational mesh of the combustion chamber is shown in Figure 2. The combustion chamber was modeled using a 45° sector mesh with periodic boundary conditions at the sector faces so that the fluid dynamics and combustion of only one diesel spray in the 8-hole injector were computed. The major geometric features of the combustion chamber – including the bowl geometry and the squish and crevice regions – were modeled in the computational mesh using the specifications of the optical engine (see Table 1). The mesh was composed of approximately 110,000 cells at bottom-dead-center (BDC), with a cell size of about 1 x 1 x 1.5 mm at the piston-bowl wall. A mesh snapping routine removed layers of cells above the piston bowl as the piston traveled towards TDC, maintaining the cell size throughout the combustion cycle simulation.

Computations were initialized from intake valve closure (IVC) with a uniform air charge in the cylinder and an initial wheel-flow velocity-profile with a swirl ratio of 0.5. The pressure at IVC was initialized based on the experimental pressure trace, and the IVC temperature was calculated assuming isentropic compression from BDC to IVC. The cylinder and piston surfaces were initialized with constant temperature boundary conditions. The fused silica piston-bowl temperature was estimated at 500 K and the cylinder wall and firedeck surfaces were estimated by increasing the initialized surface temperatures from the engine coolant temperature (98 °C) until the motored compression and expansion stroke pressures were in agreement (resulting temperature of 430 K). Note that these temperature estimates are in close agreement with predicted surface

temperatures from finite-element heat transfer computations of this engine and operating condition (approximately 510 K along the piston-bowl surface and 385 K at the cylinder head) [39]. Finally, the injection velocity profile was taken from the experimentally measured injection rate [40].

RESULTS AND DISCUSSION

The results are presented as a time sequence through important stages of the combustion process. First, experimental measurements of cylinder pressure, apparent heat-release rate (AHRR) and soot luminosity illustrate the combustion events that naturally divide the time sequence of this late-injection LTC operating condition. These results also provide a first look at the effects of spray targeting on the global combustion characteristics of this operating condition. Second, experimental PLIF images and computational predictions are compared and discussed for each phase of the combustion process, with a more detailed examination of the influence of spray targeting on in-cylinder mixing, combustion and pollutant-formation processes. To aid in this analysis, the models are used to quantitatively evaluate these processes and to examine the in-cylinder processes outside of the experimental field-of-view limitations. Finally, we close with an evaluation of each of the spray-targeting strategies, outlining the potential benefits and drawbacks on their application for late-injection LTC operating conditions.

MEASURED CYLINDER PRESSURE, APPARENT HEAT RELEASE AND SOOT LUMINOSITY - Figure 3 shows the measured cylinder pressure, AHRR, soot luminosity and injection profile for the late-injection LTC operating condition (Table 2) for the three different spray-targeting strategies investigated. The pressure data are ensemble-averaged over approximately 360-400 fired cycles from multiple runs. Four periods of the combustion cycle correlate with important phases of the combustion process and are identified at the top of Figure 3.

1. **Ignition Dwell:** A 2.25-CAD-long dwell period from the end of injection (at 6.75° ATDC) to the start of second-stage ignition near 9° ATDC allows for fuel-air premixing to occur prior to the start of main combustion. Starting prior to the end of injection, the first-stage or “cool-flame” ignition reactions cause the first “bump” in the AHRR, which accounts for approximately 5% of the total heat release.
2. **Main Premixed Burn:** Near 9° ATDC, a steep rise in AHRR signals the main premixed burn, when the second-stage ignition reactions rapidly become exothermic. This second period ends near 15° ATDC when the rapid heat release is complete. The premixed burn peaks near 12° ATDC and contributes about 80% of the total heat release.

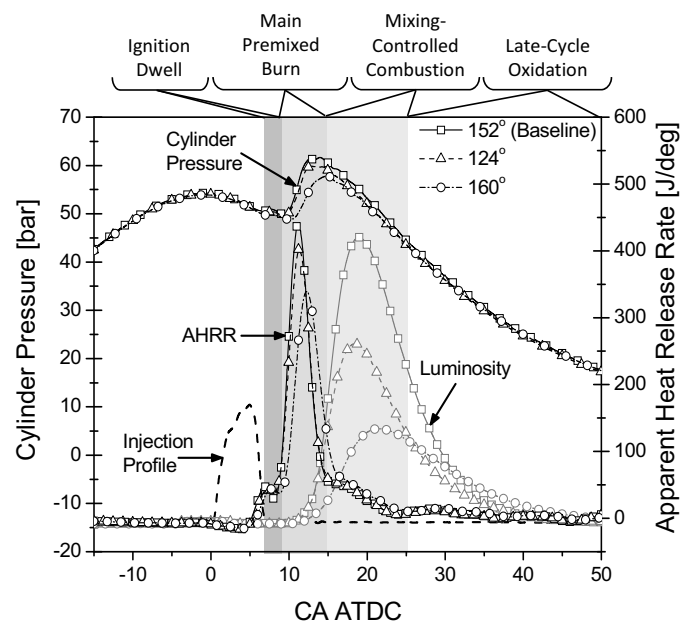


Figure 3: Experimentally measured cylinder pressure, apparent heat-release rate, volume-integrated natural luminosity and injection-rate profile for 3 spray-targeting strategies: 152° baseline spray, 124° narrow-angle spray and 160° wide-angle spray.

3. **Mixing-Controlled Combustion:** After the main premixed burn, the AHRR drops to a relatively low rate that gradually decreases from approximately 15° ATDC through 25° ATDC, during which about 15% of the total heat release occurs. This behavior is consistent with mixing-controlled combustion [41]. This period is also marked by a rise in soot luminosity, which peaks near 20° ATDC.
4. **Late-Cycle Oxidation:** After the end of mixing-controlled combustion and after the peak soot luminosity, oxidation of soot and unburned fuel continue, though the AHRR is significantly lower than during the previous three combustion periods.

As shown in Figure 3, the baseline spray angle (152°) produces the highest peak AHRR, cylinder pressure, and soot luminosity of the spray-targeting strategies investigated. In contrast, the second-stage ignition for the wide-angle (160°) spray occurs later and has a lower peak AHRR than either the narrow-angle (124°) or the baseline sprays and also has the lowest peak soot luminosity. This drop in soot luminosity can indicate decreased soot-formation levels in the wide-angle spray, as soot luminosity has been shown to correlate well with measured soot volume fraction under LTC operating conditions [13]. However, this reduction in soot may also arise primarily from the retarded ignition time that occurs with this spray targeting. With a delay in ignition, peak combustion temperatures and soot formation rates can be decreased or local equivalence ratios could be leaner due to the longer pre-ignition mixing time. Also, as discussed and explored in more detail later in the paper, soot can form in the squish regions outside of the experimental field-of-view, which can also contribute to a