

RCCI Combustion Regime Transitions in a Single-Cylinder Optical Engine and a Multi-Cylinder Metal Engine

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ABSTRACT

Reactivity Controlled Compression Ignition (RCCI) is an approach to increase engine efficiency and lower engine-out emissions by using in-cylinder stratification of fuels with differing reactivity (i.e., autoignition characteristics) to control combustion phasing. Stratification can be altered by varying the injection timing of the high-reactivity fuel, causing transitions across multiple regimes of combustion. When injection is sufficiently early, combustion approaches a highly-premixed autoignition regime, and when it is sufficiently late it approaches more mixing-controlled, diesel-like conditions. Engine performance, emissions, and control authority over combustion phasing with injection timing are most favorable in between, within the RCCI regime.

To study charge preparation phenomena that dictate regime transitions, two different optical diagnostics are applied in a single-cylinder heavy-duty optical engine, and conventional engine diagnostics are applied in a multi-cylinder, light-duty all-metal engine. Both engines are operated with iso-octane and n-heptane as the low- and high-reactivity fuels, respectively. The iso-octane fuel fraction delivers 80% of the total fuel energy, the global equivalence ratio is 0.35, and no exhaust gas recirculation is used. In the optical engine, single-shot, band-pass infrared (IR) imaging of emission near 3.3 microns measures thermal *C-H* stretch-band emission of hot fuel vapor and intermediate combustion products, providing qualitative information about the fuel-vapor distribution and ignition locations during low-temperature heat release. Additionally, high-speed 7.2 kHz visible-light imaging of natural luminosity, optimized to detect chemiluminescence, indicates the spatial and temporal evolution of high-temperature heat release and combustion. Similar combustion regimes are observed for both engine platforms, allowing an opportunity for optical engine data to provide insight into fundamental phenomena affecting regime ranges and transitions in production engines. Key findings from imaging diagnostics indicate that at the late-injection limit of RCCI control authority, low-temperature ignition occurs when clearly identifiable jet structures are still intact, and during high-temperature combustion there is prevalent and persistent soot incandescence representative of locally mixing-limited (i.e., fuel-rich) combustion. At the early-injection limit of RCCI control, observed stratification during low-temperature ignition is subtle; however, high-temperature combustion still occurs sequentially from the bowl rim radially inwards.

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INTRODUCTION

Low-temperature combustion (LTC) offers the potential for low soot and nitrogen oxide (NO_x) emissions and high efficiency, and is therefore an approach of interest for current and future engines [1]. Dempsey et al. [2] have described the typical operating space of LTC as residing within a window of the local in-cylinder equivalence ratio (ϕ) and temperature (T) space, where both soot and NO_x formation are avoided, as depicted in Figure 1.

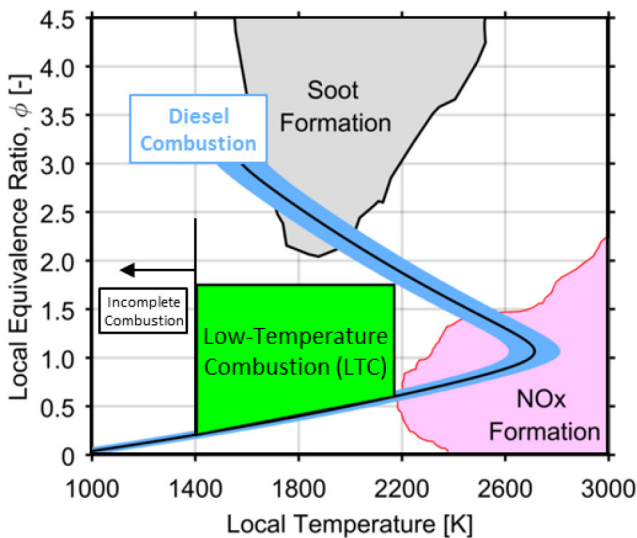


Figure 1. Low-temperature combustion region avoiding NO_x and soot formation islands in the domain of local in-cylinder equivalence ratio (ϕ) and temperature (adapted from Dempsey et al. [2]).

Operation in the ϕ - T window of LTC can be achieved by allowing sufficient time for fuel-air premixing to avoid regions of overly high ϕ , and by using dilution, either from excess air (fuel-lean mixtures) or exhaust gas recirculation (EGR), to reduce peak combustion temperatures. As a result of this approach, compression-ignition LTC modes have been shown to result in high thermal efficiencies through a combination of lean operation, optimal combustion phasing near top dead center (TDC), a short combustion duration, and reduced heat transfer [3, 4, 5, 6]. However, LTC modes also tend to suffer from high emissions of unburned hydrocarbons and carbon monoxide due to regions that are overly lean and/or too cold for complete oxidation.

Additionally, the premixing inherent to LTC implies that the combustion process is primarily kinetically-controlled, which can limit the range of stable operation [7, 8]. Uniform in-cylinder charge (i.e., ϕ and/or T) preparation results in nearly volumetric combustion, which is associated with high pressure-rise rates and combustion noise. Stratifying the ϕ and/or T within the LTC ϕ - T window by varying the timing and quantity of fuel injected can still avoid soot and NO_x formation regions while allowing for some degree of

control over the phasing and rate of combustion [9, 10, 11]. A review of the methods and implications of various approaches to achieving charge stratification is given in Dempsey et al. [2].

Dual-fuel modes can achieve control authority over combustion phasing and duration by controlling both global fuel reactivity and in-cylinder stratification of mixture reactivity due to differences in fuel composition, both physical and chemical [12, 13]. In general, the low-reactivity fuel is well-mixed prior to combustion, while the degree of premixing for the high-reactivity fuel is adjusted to control combustion. With direct injection of the high-reactivity fuel, its premixing can be controlled by varying the start of injection timing. If the direct injection is sufficiently early that both fuels are premixed before autoignition, the resulting dual-fuel combustion mode is essentially homogenous charge compression ignition (HCCI) [3]. If the direct injection is very late, typically near TDC, the resulting dual-fuel combustion mode is at least partially mixing-controlled [14, 15, 16, 17, 18]. Combustion for such late-injection conditions thus share some aspects of conventional diesel combustion, and with some amount of premixed combustion in the low-reactivity fuel, they are akin to dual-fuel diesel-pilot combustion. Between these two extremes lies a range of combustion called reactivity-controlled compression ignition (RCCI), in which the charge is sufficiently premixed to be kinetically-controlled, but also has sufficient stratification of reactivity to allow control over the combustion phasing by modulating the direct-injection timing and quantity of the high-reactivity fuel [19]. One defining feature of RCCI is a range of “control authority”, where the direct-injection timing of the high-reactivity fuel can be adjusted to control combustion phasing. Some recent work has focused on developing real-time, closed-loop control algorithms to utilize the range of this control authority for practical implementation of RCCI [20, 21].

The early- and late-injection transitions at the edges of the control authority range have been observed for a variety of combinations of low- and high-reactivity fuels. The role of fuel properties on the control authority within the RCCI regime has been investigated to some extent in single- and multi-cylinder metal engine experiments, but the fundamental physical and chemical processes dictating the location of the transitions are not well understood [22, 23, 24, 25].

Previous optical-engine studies have focused on using chemiluminescence and fuel-tracer planar laser-induced fluorescence (PLIF) imaging to better understand in-cylinder mixing and ignition processes during RCCI by identifying ignition locations and characterizing fuel stratification [26, 27, 28, 29]. Quantitative mixing measurements using PLIF are typically limited to non-combusting conditions due to uncertainties related to oxygen quenching of fuel-tracer fluorescence. A challenge remains in quantifying local fuel-air mixture compositions at the start of ignition under combusting conditions.

The present study uses two imaging diagnostics under reacting conditions, each directed at a different wavelength band. The first is blue-filtered visible natural luminosity (NL) imaging, which aims to capture chemiluminescence emission between about 380 and 500 nm arising from small excited-state intermediate combustion species such as CH_2O^* , CH^* , and C_2^* , as well as the CO continuum. Strong visible chemiluminescence is emitted during the high-temperature heat release (HTHR) stage of combustion [29, 30, 31]. The second diagnostic is filtered infrared (IR) imaging, which uses a 400-nm wide bandpass filter centered near 3.3 microns to capture thermal emission from $C-H$ stretch-band emission of hot hydrocarbons (e.g., fuel) and other species with $C-H$ bonds (e.g., large intermediate species) [32]. This 3.3-micron IR emission is present whenever $C-H$ bonded species are hot, including conditions where:

1. premixed fuel is compression-heated during the compression stroke
2. fuel is injected into and mixed with compression-heated in-cylinder gases
3. the local temperature increases during first-stage ignition low-temperature heat release (LTHR) of two-stage-ignition fuels
4. the local temperature increases in the beginning phases of high-temperature heat release when $C-H$ -bonded emitters are still present

In order to isolate chemical (i.e., autoignition) effects from physical fuel property effects, primary reference fuels (PRFs) are chosen as surrogates. Iso-octane (PRF100) is used to represent low-reactivity gasoline-type fuels and n-heptane (PRF0) is chosen to represent high-reactivity diesel-type fuels. This allows the creation of in-cylinder reactivity gradients with little impact from small differences in physical properties (e.g., density, viscosity, etc.). Neat iso-octane is used as the well-mixed fuel, and neat n-heptane as the partially-premixed fuel. The focus is on understanding underlying phenomena that dictate transitions into and out of the range of control authority.

The observations from single-cylinder, heavy-duty, optical-engine experiments at Sandia National Laboratories (SNL) are compared to experimental results from a multi-cylinder, light-duty, metal engine with conventional engine diagnostics at Oak Ridge National Laboratory (ORNL). Both engines are operated with iso-octane and n-heptane as the low- and high-reactivity fuels, respectively. The start of injection command for n-heptane ranges from 260 to 335 CAD (100 to 25 CAD before TDC), which covers the entirety of the RCCI regime with favorable control authority. The premixed-fuel (iso-octane) fraction is fixed at 80% of the total fuel energy with a global equivalence ratio of 0.35, and with no EGR. Conventional engine-performance metrics evaluated for the all-metal engine include efficiency, emissions, and heat-release rate analysis. Similar combustion mode regimes are observed in the two engines, even though they have different combustion chamber geometries, engine speeds, and number of cylinders. Selected results from the ORNL metal engine experiments are presented in this study to help provide context and demonstrate commonalities with the SNL optical engine.

These optical- and metal-engine experiments are part of a larger study, the Co-Optimization of Fuels and Engines (Co-Optima) initiative, sponsored by the United States Department of Energy (US DOE). An over-arching goal of Co-Optima is to better understand fuel-property and engine-design effects on combustion so that automotive transportation efficiency can be improved. In the context of RCCI, one focus is to isolate physical fuel property effects from chemical properties of each fuel on combustion, including regime transitions.

EXPERIMENTAL SETUP

Oak Ridge National Laboratory Multi-Cylinder Engine

The metal-engine study at ORNL uses a 2007 GM 1.9L light-duty automotive diesel engine. A detailed explanation of the experimental setup and methodology is available elsewhere [33]; a brief summary is provided here for comparison to the optical engine experiments featured in the present work. Geometric specifications for the ORNL engine are provided in Table 1, and an illustrative overview of the engine, fuel system, and air-handling layout is shown in Figure 2. The fuels are introduced into the engine through two different fuel systems. A common-rail (CR) direct-injection (DI) fuel system, which uses the stock CR injection hardware, delivers the high-reactivity (n-heptane) fuel. A port fuel injection (PFI) system, which uses an aftermarket PFI rail and injectors that are mounted to the intake manifold, delivers the low-reactivity (iso-octane) fuel. Specifications of the CR injectors are given in Table 2.

Table 1. Specifications of ORNL 2007 GM 1.9 L multi-cylinder diesel engine.

Number of cylinders	4
Bore [mm]	82.0
Stroke [mm]	90.4
Connecting rod length [mm]	145.4
Displacement [L]	1.91
Geometric compression ratio	17.5:1
IVO [°CA]	704
IVC [°CA]	228
EVO [°CA]	476
EVC [°CA]	20
Rated power [kW]	110
Rated torque [Nm]	315

Table 2. ORNL common-rail direct injector specifications.

Model	Bosch CRI 2.2 (solenoid-actuated)
Number of holes	7
Hole size [mm]	0.140
Included spray angle [deg]	148
Tip geometry design	mini-sac

The experimental conditions for the ORNL metal-engine experiments are given in Table 3, and properties of the fuels are provided in Table 4. This sweep of CR start of solenoid energizing (SSE) timing was chosen because it extended beyond both ends of the control authority range, such that the transitions into either highly premixed or highly mixing-limited combustion were clearly identified. These conditions also yielded a reasonable compromise between noise, combustion phasing, and combustion stability throughout the range investigated.

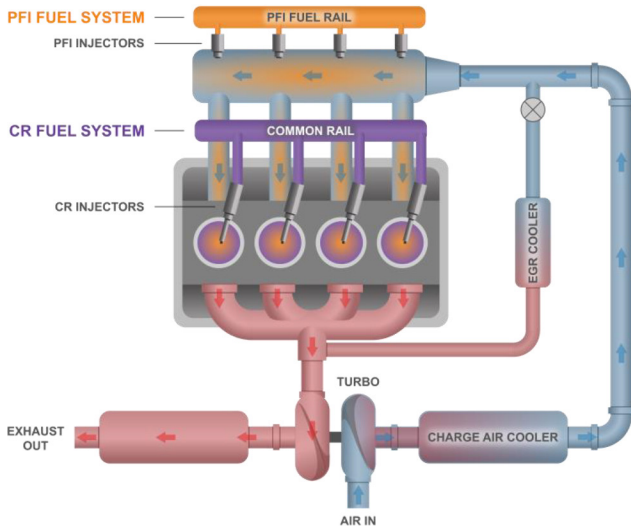


Figure 2. Diagram of the ORNL multi-cylinder all-metal light-duty GM 1.9 L engine.

Table 3. Experimental conditions for the ORNL light-duty multi-cylinder metal engine.

CR fuel	n-heptane
PFI fuel	iso-octane
Global PRF [% by vol.*]	80
CR SSE [°CA]	Start = 180 or stability limit End = PPRR ⁺ limit (>15 bar/°CA) or combustion efficiency limit (<80%)
CR fuel pressure [bar]	450
Engine speed [RPM]	2000
Mean piston speed [m/s]	6.0
Global ϕ (total fuel) [-]	0.35 (No EGR)
Total fuel rate [J/cyc]	2100 (525 J/cyl)
Nominal BMEP [bar]	~ 3.25
Nominal gIMEP [bar]	~ 4.7 (averaged)
Intake temperature [°C]	40
Intake pressure [bar]	~ 1.04
Air rate [g/s]	~ 35 (8.75 g/cyl)
EGR [%]	0

* Values on a mass, volume or energy basis are within 0.3%.

⁺ Peak pressure rise rate

Table 4. Fuel properties.

	iso-octane (PRF100)	n-heptane (PRF0)
Formula	C ₈ H ₁₈	C ₇ H ₁₆
RON	100	0
MON	100	0
Cetane Number	11-19	53-54
Lower Heating Value [kJ/g]	44.6	44.3
Stoichiometric AFR [g/g]	15.03	15.08
Boiling Range [°C]	99.30	98.38
Density [kg/m ³]	688	684
Heat of Vaporization [kJ/kg]	307	362
Viscosity [mPa·s]	0.473	0.389
Surface Tension [mN/m]	18.77	20.30

Sandia Optical Engine

The optical engine is a single-cylinder version of the Cummins N14. Engine geometry details are specified in Table 5. As shown in Figure 4, an extended (Bowditch) piston provides imaging access to the combustion chamber through a flat-bottom fused-silica piston-crown window. The engine is also equipped with a window inserted in the cylinder head in place of one of the exhaust valves to provide imaging access to the squish region, but for reasons that will be described later, the combustion-chamber surface of this window is painted black, and is thus not available for imaging in the current experiments.

Whereas the ORNL metal engine uses a PFI system to deliver the premixed fuel, the SNL optical engine uses a gasoline direct injection (GDI) system with a side-mounted (i.e., in the cylinder wall) injector to deliver the premixed fuel, as depicted in Figure 4. Specifications for the GDI system are included in Table 5. The GDI fuel is introduced as early in the compression stroke as possible with SSE at 60 °CA¹, shortly after the top of the piston has descended below the elevation of the injector. A well-mixed charge of iso-octane and air is confirmed with IR imaging of hot fuel vapor late in the compression stroke, as will be shown in the results section. Relative injection timings for both engines are shown graphically in Figure 3.

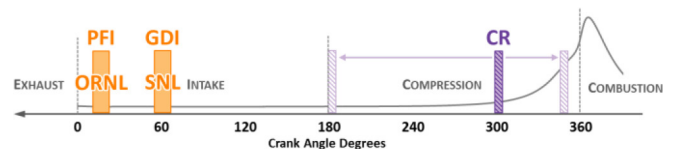


Figure 3. Injection strategies used in the ORNL and SNL experiments.

For delivery of the high-reactivity n-heptane fuel, the SNL optical engine uses a Delphi DFI-1.5 light-duty CR injector, which is similar to the CR injector in the ORNL metal engine (compare Table 2 and Table 5).

Table 5. Engine and fuel injection specifications for the SNL single-cylinder heavy-duty optical diesel engine.

Engine specifications

Displaced volume [L]	2.34
Stroke [mm]	152.4
Bore [mm]	139.7
Bowl diameter [mm]	97.8
Squish height [mm]	5.5
Compression ratio	11.22:1
Swirl ratio	~ 0.5
Intake valve open [°CA]	703
Intake valve close [°CA]	195
Exhaust valve open [°CA]	485
Exhaust valve close [°CA]	27
Skip fire ratio (motored:fired cycles)	9:1
Engine speed [RPM]	1200
Mean piston speed [m/s]	6.1
Intake temperature [°C]	~ 92
Intake pressure [bar]	~ 1.30
EGR [%]	0
Nominal gIMEP [bar]	5.5 – 5.7

Fuel injection specifications

GDI fuel injector	Bosch
GDI hole pattern	7, asymmetric (downward toward piston bowl)
GDI fuel supply pressure [bar]	100
GDI fuel	iso-octane (PRF100)
GDI SSE [°CA]	60 (during intake)
GDI DSE [ms]	6.5
CR fuel injector	Delphi DFI-1.5 (solenoid-actuated)
CR rail pressure [bar]	800
CR DSE [ms] (and approximate [CAD])	0.738 (5.3)
CR fuel	n-heptane (PRF0)
CR injector number of holes	8
CR hole size [mm]	0.131
CR included spray angle [deg]	156
CR tip geometry design	mini-sac
Global PRF [% by vol. *]	80
Global ϕ (total fuel) [-]	0.35
Global ϕ for iso-octane only [-]	0.28

* Values on a mass, volume or energy basis are within 0.3%.

It is impossible to match all operating conditions between the metal ORNL engine and SNL optical engine. The highest priority is put on variables relevant to local mixing, ignition and combustion behavior. To this end, both SNL and ORNL engines are operated with the same

global equivalence ratio and global PRF, where global PRF is computed as the sum of premixture fraction (80% of PRF100) and CR injection fraction (20% of PRF0), by volume. These values have a significant effect on local mixture preparation and the resultant fuel and reactivity gradients, to which RCCI combustion is highly sensitive. In addition, we chose to match the in-cylinder charge density and temperature at 305 °CA, which for CR SSE is roughly the midpoint of the range of control authority over combustion phasing for the ORNL engine data. This seemed the best compromise for matching in-cylinder thermodynamic conditions. To achieve this, the SNL engine intake draws undiluted, pre-heated, dry air at 92 °C and 130 kPa. This results in an estimated motored TDC core-gas conditions of 14.5 kg/m³, 37 bar and 883 K, calculated for an isentropic compression using the measured cylinder pressure.

With the global equivalence ratio and thermodynamic conditions at a particular point in the compression stroke (305 °CA) fixed, the two engines with different compression ratios have slightly different loads: 4.2-5.0 bar gIMEP for the metal engine and 5.5-5.7 bar gIMEP for the optical engine. It is noted, however, that this difference in load as quantified by gIMEP is largely a matter of normalization, related to the difference in compression ratios. That is, the chemical energy content normalized by *in-cylinder volume at 305 °CA* is the same for both engines, even if the work output normalized by *displaced volume* (i.e., gIMEP) is different.

One other important difference between the ORNL and SNL engines is the engine speed (2000 RPM and 1200 RPM, respectively). One consequence of the difference in engine speed is that chemical reactions, which proceed based on physical time, will not agree in crank angle space. While this is true, mean piston speeds are nearly matched (~ 6 m/s for both engines) which is important for creating similar turbulence characteristics (and hence mixing environments), as is common practice for scaling engines of different sizes.

The gain curve of the Bosch GDI injector was measured with a Max Machinery (model P213) piston flow meter, with the injector mounted to the engine, which was heated to normal operating conditions. The gain curve and injection rate for the CR Delphi DFI-1.5 injector were measured with a custom force-transducer-based rate-of-injection meter [34]. The duration of solenoid energizing (DSE) for each injector is listed in Table 5.

Finally, the optical engine is skip-fired to avoid excessive temperature gradients within the engine windows that would cause them to fracture. For each experimental test run of the optical engine, the engine was skip-fired, with each fired cycle followed by nine motored cycles to allow steep temperature gradients generated during combustion to relax to tolerable levels before the next fired cycle. After a start-up transient of motoring for 60 seconds, a total of 40 skip-fired cycles were acquired. The associated cylinder pressure traces are post-processed by applying a low-pass filter with a Gaussian roll-off function having a transmission of 100% from 0 to 800 Hz and dropping to 1% at 3360 Hz, and then used to compute the apparent heat release rate (AHRR) for each fired cycle using standard techniques [35].

Optical Setup - Visible Natural Luminosity Imaging

Two different digital cameras are used for simultaneous imaging of ignition and progression of combustion. As shown in Figure 4, a dichroic beamsplitter separates visible from IR emission, and directs each spectral band to two different cameras. The beamsplitter reflects light at the blue end of the visible-light spectrum, and transmits light of green and longer wavelengths, through much of the near- and mid-IR. The cutoff wavelength varies from 90% reflectance at 466 nm, 50% at 490 nm, and to 25% at 530 nm. A high-speed, 14-bit CMOS monochromatic camera (Phantom model v7.3) images the visible-light emission reflected from the beamsplitter, and is triggered once per CAD, or approximately 7.2 kfps at 1200 RPM, using shaft encoder pulses. The exposure time is fixed at 130 microseconds, which corresponds closely to the 139 microsecond duration of one full CAD at 1200 RPM. This exposure time was chosen to be sensitive enough to observe chemiluminescence, while avoiding significant pixel blooming during saturation under high-luminosity conditions (i.e., due to soot incandescence). The blue-filtering of the beamsplitter further reduces the strong longer wavelength emission from soot incandescence.

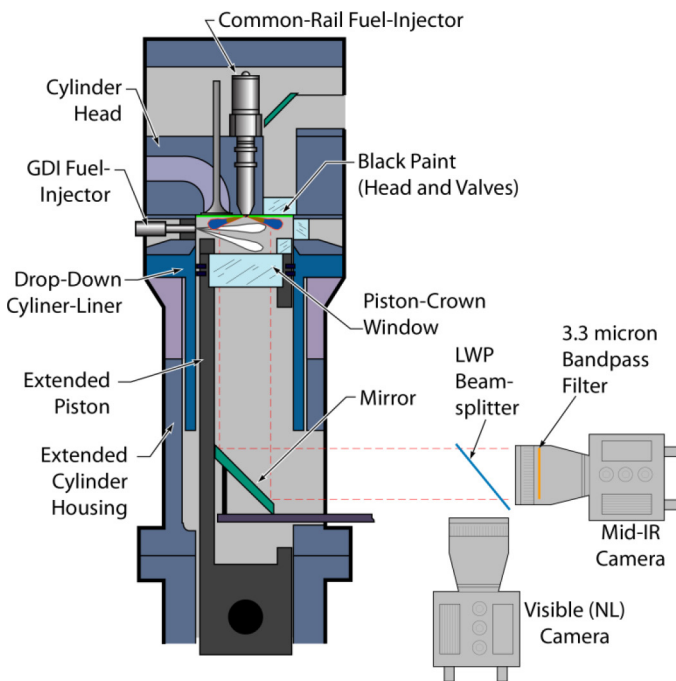


Figure 4. Sandia single-cylinder heavy-duty optical engine.

Optical Setup - 3.3-Micron IR Imaging

The IR light transmitted through the beamsplitter is bandpass-filtered at 3.3 microns with a full-width at half-maximum (FWHM) of 430 nm (Spectrogon BP-3317-215). This spectral range is specifically aimed to capture thermal emission arising from the *C-H* stretch band, for which the intensity is a function of both *C-H* bond concentration and temperature [36, 37]. This filter is housed behind the lens within a filter wheel, attached to the infrared camera (Telops, 16-bit InSb array). When using the full array, the maximum frame rate is 340 Hz, which limits the temporal resolution per cycle to about 1 frame every 20 CAD at 1200 RPM. Hence, for the limited crank-angle range of interest during combustion, relevant images from the IR camera can

only be acquired once per fired cycle. Ten different specific crank angle positions are chosen to focus on LTHR and HTHR periods. With a total of 40 fired cycles, this results in 4 available images per crank angle position for each engine run. Images have an exposure time of 130 microseconds, which yields an IR image with acceptable signal to noise, and also matches the exposure time of the visible-light camera to facilitate direct comparison of simultaneous images.

One challenge of measuring IR emission from within the optical engine is due to reflections off of the cylinder head. Early experimentation produced IR images with obvious variations in reflectivity across the surface of the firedeck. This created a measured intensity that was a function of the combined desired direct IR emission and variable reflected emission. To yield a more uniform image with low reflectivity, and to help simplify the image analysis, a high-temperature-suitable black paint is applied to the head surface, without the injector installed. This coating of paint significantly reduces reflection of IR emission from sources within the cylinder during compression and combustion.

To illustrate the difference between a variable-reflectivity un-coated cylinder-head firedeck and using black, relatively uniform low-IR-reflective paint, Figure 5 shows two images of a relatively homogeneous fuel charge acquired before and after painting. These images correspond to using a GDI iso-octane injection only, with the same intake conditions, and are taken at the same crank-angle position.

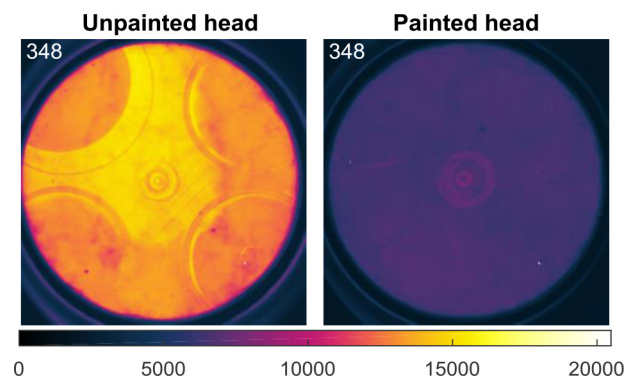


Figure 5. 3.3-micron IR images with GDI iso-octane injection only. Exposure time is 130 microseconds. Observable features in the leftmost image include valve edges, injector tip, and head surface scratches. CAD for each image are shown in the upper left corner. Full well-depth corresponds to 65,536 counts.

The image gain in Figure 5 is the same for both images, and was chosen such that the 'unpainted head' image on the left remains just below saturation. The mean intensity is about 13,500 counts for the unpainted firedeck (left), and about 6,500 counts with the painted firedeck (right). Without the black paint, many features of the engine head surface are apparent, such as the centrally-mounted injector and its annular adapter, the outlines of two intake and one exhaust valve, and the dark low-reflectivity surface of the cylinder-head window and its mounting adapter (top-left corner). Furthermore, the captured intensity is non-uniform, for instance with dark areas between the valves at the bottom and right, but bright areas at the top and left of the image. This non-uniformity is attributed to differences in the build-up of soot on the firedeck. The center and top-left areas of the firedeck have been frequently cleared for optical diagnostic purposes

associated with the cylinder head window in the upper-left corner. Non-uniformity is also apparent in visible-light images, but to a much lesser degree than in the IR. Apparently, the difference between reflectivity of clean cast iron and soot deposits is much greater in the IR than for visible light. Although it is conceivable that image post-processing could correct for small differences in reflectivity, we elected to try using a painted surface. With the painted surface, reflections are reduced greatly, and the image is much more uniform than without a painted surface. Certain observable features remain even in the painted image, however, namely the injector tip, injector adapter annulus, and a few regions around valve edges. These are areas that lost black paint during experimentation, and are now viewable due to reflection of the fuel-vapor IR emission off those now unpainted surfaces.

SINGLE-ZONE IC ENGINE MODEL

To help interpret the optical data, a single-zone, time-dependent, 0-D internal combustion engine model is implemented using Chemkin-Pro with the kinetic mechanism of Curran et al. for n-heptane and iso-octane, consisting of 1034 species and 4238 reactions [38, 39]. The engine model uses the built-in crank-slider model of the Chemkin-Pro package, initialized with geometric parameters and operating conditions from the experiment.

The initial gas composition for each simulation is set to represent local experimental conditions. The ratio of iso-octane to air is held constant to represent the well-mixed, early GDI injection. To this mixture, quantities of n-heptane are added to analyze different hypothetical local PRF mixtures. A range of initial compositions and the associated PRF and ϕ values are in Table 6. As will be discussed in the results section, because of the heterogeneous distribution of the CR injection of n-heptane, key igniting mixtures are expected to be above the global ϕ and PRF, i.e., locally $\phi > 0.35$ and $\text{PRF} < 0.80$. Hence, the mixtures in Table 6 are richer and have lower PRF than the global values, with the exception of the bottom row for the GDI-injection of iso-octane only, which is included as a reference point.

Table 6. Engine model input mole fractions of PRF species and air.

PRF	ϕ	i-C ₈ H ₁₈	n-C ₇ H ₁₆	O ₂	N ₂
20	1.306	0.00472	0.01889	0.2043	0.7721
30	1.133	0.00476	0.0111	0.2059	0.7783
40	0.670	0.00478	0.00717	0.2067	0.7813
50	0.543	0.00479	0.00479	0.2072	0.7832
100	0.289	0.00481	0	0.2082	0.7870

The estimated initial BDC temperature and pressure in the optical engine are 95 °C and 145 kPa, slightly different conditions than those measured from the intake runner as reported in Table 5. Additionally, a heat loss model using the Woschni correlations [40] is included.

Band-integrated absorption cross-sections of gaseous species with C-H bonds, such as iso-octane, n-butane, propane, and ethanol, have relatively high sensitivity in the 3.1-3.5 micron band [36]. By assuming thermal equilibrium and applying Kirchhoff's Law, there is a

corresponding emission in the same band. This emission is attributed in large part to C-H bond vibrational transitions [37]. Furthermore, the absorption cross-section is approximately proportional to the number of C-H bonds in the molecule [36]. The single-zone engine model results can be useful for predicting the total number of C-H bonds, integrated over all of the species present, that exist at any given time during ignition and combustion. Contributions from trace species below 0.1 ppm mole fraction are negligible and not included in the computation.

In the optically thin limit (negligible signal trapping), thermal IR radiation from C-H stretch emission is proportional to both the number density of C-H bonds and to the blackbody radiation within the emission band at the local gas temperature. Within a given image, for which the pressure is relatively uniform, the local number density is inversely proportional to gas temperature according to the ideal gas law. The resultant proportionality relationship between C-H bond emission sources and expected relative intensity of emission is given by:

$$I_{IR,thin} \propto \frac{X_{CH} \cdot I_{bb}(T, 3.3 \text{ micron})}{T} \quad (1)$$

where $I_{IR,thin}$ is the IR emission intensity in the optically thin limit, X_{CH} is the mole fraction of C-H bonds, T is the local gas temperature, and $I_{bb}(T, 3.3 \text{ micron})$ is the blackbody radiation intensity at T and a wavelength of 3.3 microns.

RESULTS AND DISCUSSION

Heat Release Rate and Combustion Phasing

The ensemble-averaged AHRR data for the range of CR SSE timings of n-heptane injection in the optical engine are shown in Figure 6. The actual start of injection (i.e., the emergence of fuel from the injector orifices) occurs about 3 CAD after SSE due to electrical and hydraulic delays.

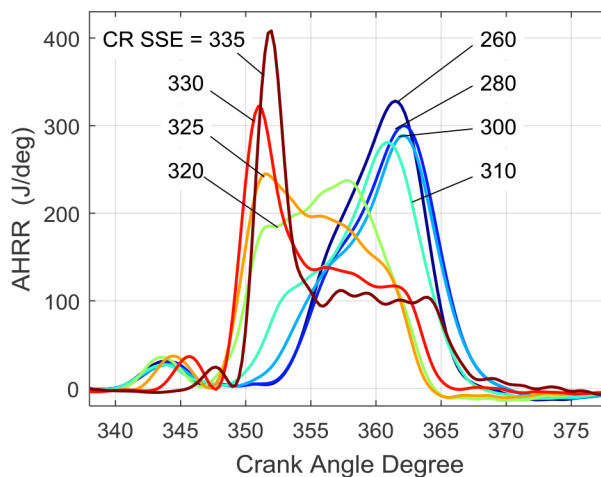


Figure 6. SNL optical engine ensemble-averaged (from 36 cycles) AHRR for various CR SSE timings (in °CA), with TDC of compression at 360 °CA. Global PRF = 80 and global $\phi = 0.35$. Nominal intake conditions are 92 °C and 130 kPa.