

Investigation of the Combustion Front Structure during Homogeneous Charge Compression Ignition Combustion via Laser Rayleigh Scattering Thermometry

Matthew Blessinger and Jaal Ghandhi
University of Wisconsin

ABSTRACT

The combustion propagation mechanism of homogeneous charge compression ignition combustion was investigated using planar laser Rayleigh scattering thermometry, and was compared to that of spark-ignition combustion. Ethylene and dimethyl ether were chosen as the fuels for SI and HCCI experiments and have nearly constant Rayleigh scattering cross-sections through the combustion process. Beam steering at the entrance window limited the load range for HCCI conditions and confined the quantitative interpretation of the results to local regions over which an effective beam steering correction could be applied. The SI conditions showed a clear bimodal temperature behavior with a well-defined interface between reactants and products. The HCCI results showed large regions that were partially combusted, *i.e.*, at a temperature above the reactants but below the adiabatic flame temperature. Dual-imaging experiments confirm that the burned region was progressing towards the fully burned state. This suggests that combustion is a distributed (spatially) ignition process. There were, however, a significant number of regions of the HCCI temperature field that had relatively steep temperature gradients, which could signify the presence of a local laminar flame structure. Thus, it appears that both combustion modes are contributing to the combustion propagation mechanism for HCCI combustion.

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INTRODUCTION

With future pollutant emission and fuel economy regulations becoming stricter, it is imperative to develop internal combustion engines that can meet the current standards and still retain room for improvement to meet future mandates. Gasoline engines have made rapid improvements in recent years through a combination of advanced fuel injection hardware (direct injection) and boosting technology, but unburned hydrocarbon (UHC), nitric oxide (NOx) and carbon monoxide (CO) emissions are still an issue that requires aftertreatment which reduces the system efficiency [1,2]. Conventional diesel combustion operating unthrottled, globally lean and with high compression ratios achieves high thermal efficiency with low CO and UHC emissions [3] but has high NOx and soot formation due to the structure of the lifted diesel flame [4]. Like gasoline engines, diesel engines require aftertreatment systems such as a diesel oxidation catalyst, diesel particulate filter and selective catalytic reduction to be sold in the current emission-constrained marketplace.

Advanced engine technologies are being pursued to improve efficiency while reducing engine-out emissions, hopefully to a level low enough to eliminate the costly, complex aftertreatment systems. Low-temperature combustion (LTC) strategies utilize both high dilution levels to maintain low-temperatures and, consequentially, low NOx formation, and mixtures lean enough to avoid soot formation. Both goals can be achieved by diluting with air, or in many cases, recirculated exhaust gas (EGR). One of the most

researched LTC strategies is homogeneous charge compression ignition (HCCI) combustion, where an overall lean, homogeneous fuel-air mixture autoignites nearly simultaneously. When short heat release is properly phased, high thermal efficiency combustion is achieved with ultra-low soot and low NOx [5, 6, 7].

Despite being one of the longest researched LTC combustion regimes, the exact mode of combustion propagation in HCCI remains an outstanding issue. In principle, for a homogeneous mixture the entire charge would simultaneously ignite. In reality, the combustion event is short, it typically takes ~5 crank angle degrees, which corresponds to <1 ms at road cruising speeds [8]. Combustion in an SI engine takes on the order of 40-60 crank angle degrees [3], corresponding to a duration of ~6 ms. With HCCI's combustion event being much shorter than that of flame propagation, the mechanism of the propagation is usually assumed to be sequential autoignition. The only known publication to attempt to prove that an autoignition front existed was done by Hasegawa *et al.* [9], in which 2-D phosphor thermometry measurements were made to map the temperature profile across a combustion front. The authors classified the combustion as purely autoignition due to 1-3 mm combustion front length scales, but the imaging resolution was too coarse to resolve flame propagation and the measurements were performed in the low-temperature chemistry regime, which is auto-ignition by nature. Overall, the measurement methodology of the Hasegawa *et al.* experiment lacked the ability to make definitive determinations about the combustion propagation mechanism.

A classification of combustion wave propagation was proposed by Zeldovich [10] and extended to HCCI combustion by Chen *et al.* [11]. Equation 1 shows the front speed, s , in terms of the ignition chemistry; $d\tau/dT$ is the ignition delay's temperature sensitivity and ∇T is the temperature gradient.

$$s = \left| \frac{d\tau}{dT} \right|^{-1} \left| \frac{1}{\nabla T} \right| \quad (1)$$

Autoignition fronts are known to be broader than a premixed flame, and as such have a shallower temperature gradient, which results in a faster combustion speed according to Zeldovich's proposal. Therefore to classify the combustion front one needs the temperature gradient at the combustion front.

Several optical techniques have been used to identify the HCCI combustion front, such as planar laser-induced fluorescence (PLIF) of a tracer species added to the fuel, PLIF of an intermediate or equilibrium combustion species, and Mie scattering. The PLIF and Mie scattering techniques can be made quantitative, in some cases, to measure the temperature, but they do not typically work across the whole combustion front, which leaves an incomplete characterization; fuel tracer species are consumed with the fuel in the early stages of the combustion front [12,13], and intermediate and equilibrium species exist for only the intermediate or end stages of combustion [14]. Temperature measurement techniques such as spontaneous Raman scattering spectroscopy or coherent anti-stokes Raman scattering have either low signal levels or are single-point measurements not allowing for a temperature gradient estimation. Phosphor-based methods have similar issues to PLIF and Mie scattering in that the phosphor particles are consumed during combustion [15]. As such, we have an incomplete picture of fundamental mechanism of HCCI combustion front propagation. This in turn limits our ability to accurately and robustly model the combustion process.

Due to the limitations of the other temperature measurement techniques, Rayleigh scattering was pursued in this study. Rayleigh scattering, which is an elastic scattering technique, originates from all the molecules in the laser path, thus no additives are required; additionally, because molecules exist before, during and after the combustion front, Rayleigh scattering radiation is produced through the whole combustion event giving the full temperature profile necessary for the determination of the temperature gradient. Fewer calibrations for temperature, pressure, and species concentration are needed to make the measurements quantitative since the scattering is elastic and proportional to the molecules' cross section and number density [16]. Rayleigh scattering was used by Smith [17] to measure the temperature gradient and flame thickness of premixed flames in an SI engine and has also been applied in engines to study mixing phenomena, *i.e.*, to study the fuel concentration field [18, 19, 20]. Pitfalls to Rayleigh scattering lie in the elastic scattering nature of the signal, though, so any extraneous light scattered from a surface, *e.g.*, the walls or liquid, is a detriment to the measurements. This requires extensive design and setup procedures to ensure the highest quality data.

The objective of the study was to investigate the structure of the combustion front in HCCI combustion. This will provide insight into the role of flame propagation and successive autoignition in the HCCI combustion front propagation, which has lacked a fundamental understanding, in part, due to the diagnostic challenge. The experiment was carried out in a firing, optical internal combustion engine by means of planar laser Rayleigh scattering thermometry. Spark-ignition experiments were performed for a baseline comparison to known flame propagation. The presented analysis is qualitative in nature with quantitative results provided when necessary.

RAYLEIGH SCATTERING

The Rayleigh scattering intensity, I_R , is given by Equation 2 where η is the optical system's collection efficiency, I_i is the incident laser intensity, N is the number density of the gas, l is the test section length, and $\partial\sigma_R/\partial\Omega$ is the differential Rayleigh scattering cross section dependent on the solid angle, Ω , subtended by the viewing optics [21].

$$I_R = \eta I_i N l \frac{\partial\sigma_R}{\partial\Omega} \quad (2)$$

Assuming an ideal gas, the scattering intensity can be written as a function of pressure and temperature. Further defining a reference condition of known thermodynamic conditions, given by the naught subscript, the governing Rayleigh scattering thermometry equation is derived, as shown in Equation 3. The optical arrangement is assumed to be unchanged between the reference and test conditions such that the collection efficiency, laser energy, test section length and solid angle are the same. The desired temperature, T , is a simple function of six variables. As presented below, the Rayleigh scattering intensities, $I_{R,0}$ and I_R , are measured with a CCD camera, and the pressures are measured with an in-cylinder pressure transducer; the unmeasured quantities left are the reference temperature and the scattering cross sections. The overbar in the cross section terms indicate the mixture-average cross section which is calculated as the molar average of all molecules in the mixture.

$$\frac{T}{T_0} = \frac{I_{R,0}}{I_R} \frac{P}{P_0} \frac{\partial\bar{\sigma}_R}{\partial\bar{\sigma}_{R,0}} \quad (3)$$

For this analysis, the reference condition was taken as the reactant side of the combustion front. The pressure was thus assumed to be constant across the front, removing the pressure ratio from Equation 3, and the equal laser energy assumption was directly satisfied. The reference temperature was calculated through isentropic relations using the intake conditions. The measurement volume was in the core of the cylinder, away from the walls, allowing reasonable approximation of the reference temperature.

Rayleigh Scattering Cross Section

The Rayleigh scattering cross section is the more complex portion of Equation 3 in that it is dependent on several factors such as the wavelength of incident light, λ , index of refraction, n , depolarization ratio, $\rho_p(\lambda)$, which is wavelength dependent and the observation angle relative to the incident light polarization, ϕ . Equation 4 shows the form of the differential cross section implemented with the Loschmidt number denoted by N_0 . The scattering cross section is obtained by integrating the differential cross section over the solid angle, Ω . The differential scattering cross sections were calculated with Equation 4 using experimentally obtained indices of refraction and depolarization ratios [22, 23, 24, 25]. Combustion species without experimental indices of refraction were calculated using the summation method per Jenkins and White, in which the refractive index of the individual atoms of a molecule linearly contributes to total index of refraction [26].

$$\frac{\partial \sigma_R}{\partial \Omega} = \frac{9\pi^2}{\lambda^4 N_0^2} \left(\frac{n^2 - 1}{n^2 + 2} \right)^2 \left(\frac{3 + 6\rho_p(\lambda)}{3 - 4\rho_p(\lambda)} \right) \sin^2 \phi \quad (4)$$

Examination of Equation 4 leads to several observations about Rayleigh scattering experiments. First, decreasing the incident light wavelength greatly increases the scattering intensity. In combustion experiments, the choice of wavelength has to take into account combustion luminosity and the potential for laser-induced fluorescence, as the Rayleigh scattering intensity is relatively weak in comparison. Second, the greatest scattering intensity is obtained through orthogonal observation to the incident light polarization. Lastly, the cross section is dependent on the scattering molecules via the refractive index and depolarization ratio.

Fuel Selection

Because the scattering cross section is dependent on the individual molecules, the mixture-averaged differential cross section changes with the composition across the combustion front. The differential scattering cross section increases with molecular size (via the index of refraction), so typical hydrocarbon fuels (e.g., gasoline, diesel, etc.) have much larger cross sections than the typical products of combustion (e.g., CO_2 , H_2O , etc.). Therefore the mixture cross section change across the combustion front must be accounted for in Equation 3; if the decrease is not accounted for, the resulting temperature will be over-calculated. To minimize the change in cross-section and subsequent uncertainty, smaller hydrocarbon fuels were analyzed to find a cross section ratio as close to unity as possible. Based on this analysis, ethylene (C_2H_4), a low reactivity fuel was chosen for the SI experiments and dimethyl-ether (DME, CH_3OCH_3) was chosen for the high-reactivity HCCI fuel. The same fuel could not be used for both experiments due to the disparities in operating conditions.

The cross section change due to combustion was calculated using both CHEMKIN flame propagation and Cantera ignition delay simulations. Comparison of chemical mechanisms to experimental data found a different mechanism was needed for each combustion mode and fuel to yield the best results: ethylene flame propagation

[27] and autoignition [28], DME flame propagation [29] and autoignition [30]. Figure 1 shows the calculated $\partial \bar{\sigma}_R / \partial \bar{\sigma}_{R,0}$ ratio across the combustion front for the nominal SI condition discussed below. The cross section decreases from the reactants to products due to the larger size of the fuel molecule; the reactant and product sides are clearly defined by the two steady state values. The ignition delay simulations were taken to be representative of autoignition conditions that have spontaneous and volumetric combustion. These simulations were performed for the SI experiment conditions to validate the methodology. The time axis was scaled to fit for a better comparison.

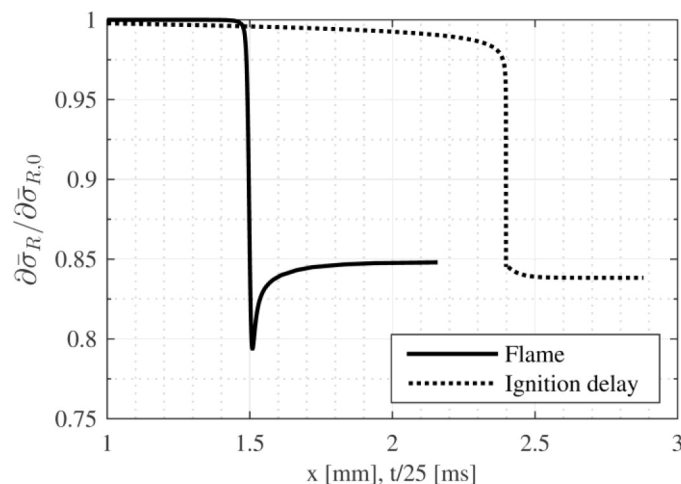


Figure 1. Cross section ratio of ethylene flame propagation and ignition delay simulations. 800 K, 13 bar, $\Phi=1.03$.

Of note is the 15% decrease in cross section between the reactant and product mixture, which ideally would be zero. It is recognized that a mixture of 38% methane + hydrogen has been used in turbulent non-premixed flames with a 2% difference between the reactant and product cross sections [31]. The mixture reactivity, however, was too low for use in the HCCI experiments with the given hardware. For the calculated adiabatic flame temperature of 2650 K in the SI experiments, the reactant-to-product intensity ratio is 3.75, which is 25x greater than the cross-section change, and the image shot-noise was of a comparable level to the cross-section change. Given the stark contrast between the reactants and products, which allows for precise identification of the reactants and products, a post-processing method was employed to account for the cross-section correction.

Owing to the low temperature chemistry of DME, Figure 2 shows two decreases in the cross section ratio for the HCCI condition. As will be shown below, the HCCI image timing was always after the low-temperature ignition event to investigate the second stage of combustion. Since the reference condition was taken as the reactant side of the combustion front at the time of imaging, the reference condition was not the supplied fuel-air mixture, but instead the post-low temperature mixture. The two curves in Figure 2 have been normalized to the post-low temperature ignition mixture of the ignition delay simulation. From this, it is observed the leaner HCCI mixture has a smaller (9.5%) decrease in the scattering cross section. It is noted that the post-low temperature mixture is different for the flame propagation

and ignition delay simulations and was accounted for in the uncertainty analysis of the Rayleigh scattering thermometry equation. Further, the mixture cross-section also continues to change in the ignition delay simulations up to the point of second stage ignition, which will add further uncertainty in determining the absolute temperature.

Comparison of the flame propagation and ignition delay simulations for the SI and HCCI cases shows the two simulation methods to be interchangeable when determining the cross section change. For the SI

conditions, there is a 1.1% difference between the product mixtures of the flame propagation and ignition delay simulations, whereas it is 0.1% for the HCCI conditions. The smaller difference than the SI case can arise from the lean conditions of HCCI combustion; a large amount of the product mixture is O_2 and N_2 regardless of the combustion mode. For stoichiometric combustion, the lack of dilution means the product mixture differences from the combustion modes are more pronounced. Furthermore, the different chemical mechanisms will produce different results.

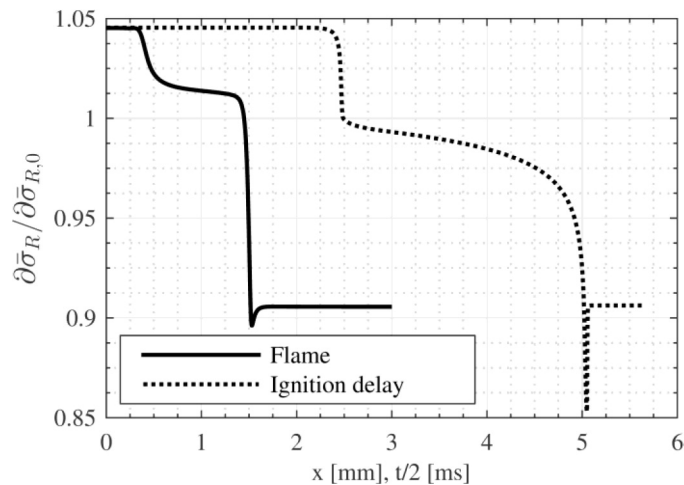


Figure 2. Differential Rayleigh scattering cross section ratio using flame propagation and ignition delay simulations for the HCCI condition 750 K, 10 bar, $\Phi=0.60$.

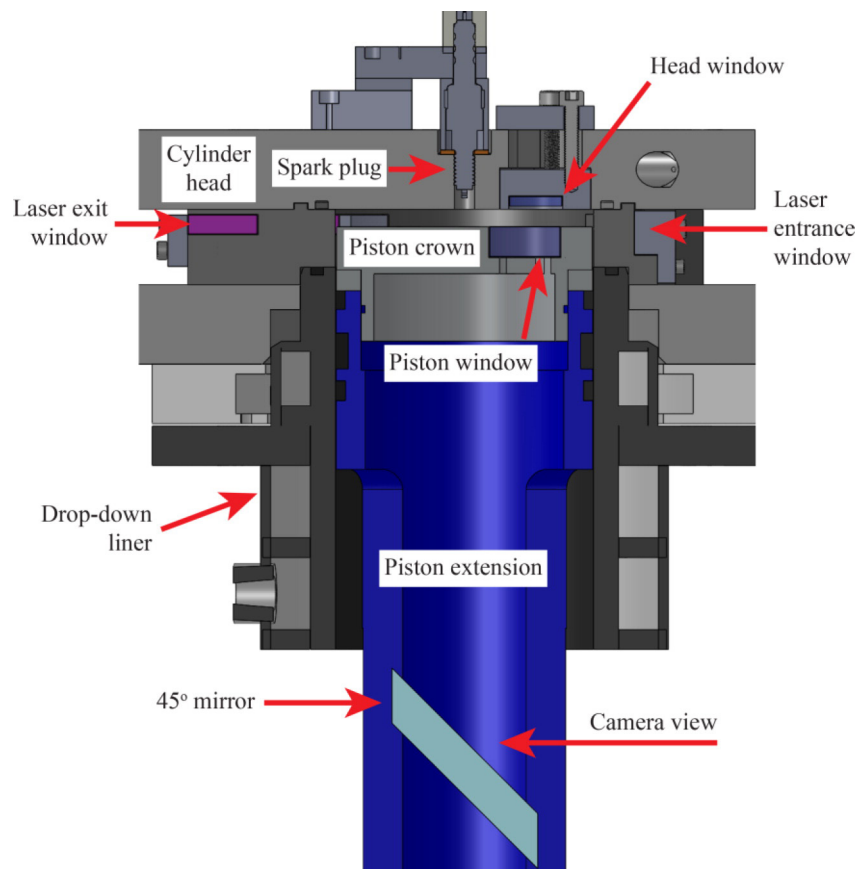


Figure 3. Optical engine assembly shown with a spark plug for SI experiments. A metal blank replaced the spark plug during HCCI experiments.

Another issue seen in the cross section ratio in the combustion front is the dip that sometimes occurs just upstream of the flame front or just before ignition timing. The width, depth or existence of the dip were not repeatable across thermodynamic or mixture conditions. Therefore to not impose unknown physics on the situation, linear interpolation between the steady-state reactant and product cross sections was performed during temperature calculations. For all experiments, the ignition delay simulations were used to estimate the cross section change across the combustion front for the SI and HCCI experiments. Any observed differences between the flame and ignition delay product values were included in the uncertainty analysis of the temperature calculations.

EXPERIMENTAL APPARATUS

Engine and Optical Access

The experiments were performed in a single-cylinder optical engine with an extended Bowditch piston as shown in [Figure 3](#). The basic engine details are listed in [Table 1](#). The engine's relatively low compression ratio of 9.0-9.6 (depending on the setup), which is not optimal for HCCI, is an artifact of the required optical setup. The engine was operated at 1200 RPM for all experiments to match the 10 Hz laser system.

Table 1. Engine geometry. Crank angle timings are relative to TDC of compression.

Displacement [L]	0.4
Geometric Compression Ratio	9.0:1 (spark-ignition)
	9.6:1 (HCCI)
Engine Speed [RPM]	1200
Squish Height [mm]	8.1 (spark-ignition)
	7.5 (HCCI)
Connecting Rod [mm]	144.8
Bore [mm]	82.4
Stroke [mm]	76.2
Exhaust Valve Open	164° ATDC
Inlet Valve Open	346° ATDC
Exhaust Valve Close	-346° ATDC
Inlet Valve Close	-164° ATDC
Swirl Ratio	0.1

The elastic nature of Rayleigh scattering makes it particularly susceptible to stray laser light that degrades the image quality. The two major stray light sources are solid surfaces and suspended particles. The squish height for both setups was increased to the extent possible to maximize the laser sheet-to-metal distance, in an attempt to minimize the amount of surface scatter off the piston, head, and all exposed metal surfaces inside the combustion chamber at TDC, which were painted with high-temperature, high-absorptivity paint. To prevent particle contamination, a high flow rate, 10 μ m filter was used upstream of the engine, and both ethylene and DME were introduced in the gaseous phase to prevent liquid droplets; the fuels were research grade purity >99.99%. An oil-less cylinder head was

used to prevent lubricating oil from entering the engine from the valve train, and a PTFE compression ring allowed oil-less operation in the engine liner.

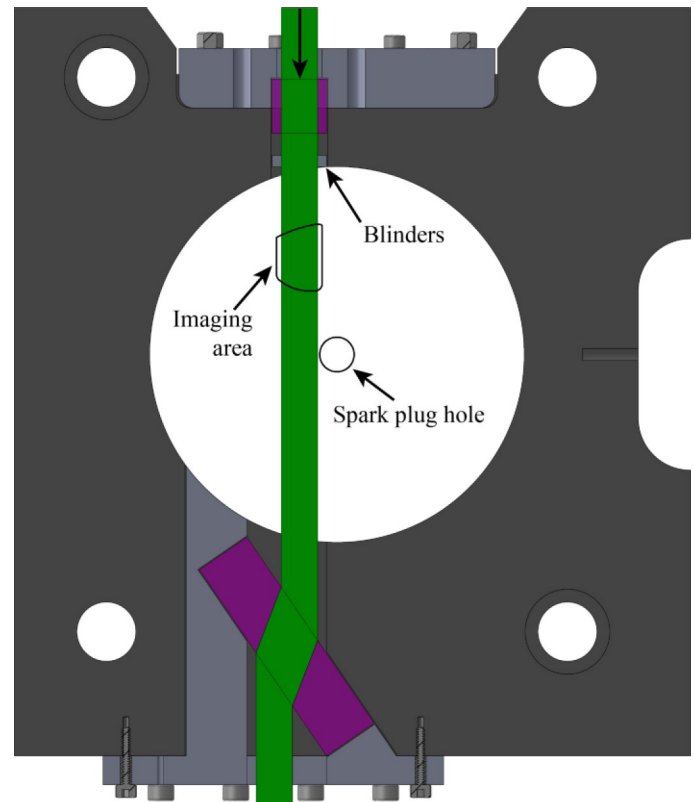


Figure 4. Overhead cutaway view of the laser-access plate. Laser-access windows are shown in purple, and the green laser path's direction is top to bottom.

Optical access was obtained through a window mounted in the piston crown at the top of the extension (see [Figure 3](#)). A 45° mirror located in the piston extension's slot allowed viewing through the piston window into the combustion chamber. A window mounted in the head provided a low-scattering background for the Rayleigh scattering measurements. Metal surfaces, regardless of the anti-reflection coating, scattered too much light that overpowered the Rayleigh scattering signal. Laser access was achieved through a plate below the head in which a pair of opposing windows allowed the laser to enter and exit the engine (see [Figure 3](#) and [Figure 4](#)). The region of interest is indicated by the black outline in [Figure 4](#); the shape is a result of the overlapping piston and head window areas. The minimal rectangular measurement area was 10.1 x 9.3 mm with its center 23 mm from the center of the cylinder.

The entrance window holder had a small aperture outside the engine to limit scatter from the sheet-forming optics from entering the engine. Both the entrance and exit windows were recessed from the cylinder bore to decrease scattered light from reaching the piston and head windows. (The recessed windows in the laser-access plate greatly contributed to the low compression ratio). Scattering from the cylinder-side of the entrance window, despite the laser-quality surface finish, was found to be significant. Accordingly, blinders were added to the cylinder-side of the entrance window channel to decrease the line-of-sight view factor between the piston, head, and entrance windows. Additionally, the exit window was recessed from the cylinder bore to decrease scatter from the sheet-forming optics from entering the engine. Both the entrance and exit windows were recessed from the cylinder bore to decrease scattered light from reaching the piston and head windows. (The recessed windows in the laser-access plate greatly contributed to the low compression ratio). Scattering from the cylinder-side of the entrance window, despite the laser-quality surface finish, was found to be significant. Accordingly, blinders were added to the cylinder-side of the entrance window channel to decrease the line-of-sight view factor between the piston, head, and entrance windows. Additionally, the exit window was recessed from the cylinder bore to decrease scatter from the sheet-forming optics from entering the engine.