

Dual-Wavelength PLIF Measurements of Temperature and Composition in an Optical HCCI Engine with Negative Valve Overlap

Jordan A. Snyder and Ronald K. Hanson
Stanford University

Russell P. Fitzgerald and Richard R. Steeper
Sandia National Laboratories

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ABSTRACT

Negative valve overlap (NVO) is a valve strategy employed to retain and recompress residual burned gases to assist HCCI combustion, particularly in the difficult regime of low-load operation. NVO allows the retention of large quantities of hot residual burned gases as well as the possibility of fuel addition for combustion control purposes. Reaction of fuel injected during NVO increases charge temperature, but in addition could produce reformed fuel species that may affect main combustion phasing. The strategy holds potential for controlling and extending low-load HCCI combustion.

The goal of this work is to demonstrate the feasibility of applying two-wavelength PLIF of 3-pentanone to obtain simultaneous, in-cylinder temperature and composition images during different parts of the HCCI/NVO cycle. Measurements are recorded during the intake and main compression strokes, as well as during the more challenging periods of NVO recompression and re-expansion. To improve measurement quality, effects of diagnostic uncertainty and fluorescence interference are quantified. Temperature, fuel, and EGR images are captured for a range of NVO operating conditions, including main and NVO fuel-injection timings as well total load. The results demonstrate that the diagnostic is capable of providing information useful for the study of HCCI/NVO engine operation.

INTRODUCTION

Development of the gasoline homogeneous charge, compression-ignition (HCCI) engine is currently focused on extending its low-emission and high-efficiency performance to a wider operating range. At the low end of the range, many strategies incorporate extensive internal exhaust gas recirculation (EGR; throughout this paper, EGR exclusively refers to *internal* exhaust gas recirculation) to enable HCCI low-load operation [1-3]. A common approach is the negative valve overlap (NVO) strategy based on injecting and reacting/reforming a small quantity of fuel during NVO recompression [4-6]. An advantage of the strategy is the potential for controlling main combustion phasing by varying NVO parameters such as the amount of EGR, the NVO injection timing, and the NVO/main fuel-injection split.

While performance of low-load NVO operation has been demonstrated, our understanding of the strategy is rudimentary. Fuel reformation during NVO provides both heat and reaction products that affect main combustion phasing. While pressure records can provide an estimate of heat release during NVO, the extent of reaction, the composition of reformed gases, and the relative importance of thermal and chemical influences on main combustion are mostly unknown. Previous optical diagnostic studies have provided some limited details of NVO chemistry such as laser-induced fluorescence (LIF) detection of formaldehyde during low-temperature reactions of two-stage fuels, and evidence of high-temperature reactions via OH chemiluminescence [7]. Our current work addresses the gap in understanding of

the NVO strategy through the development and application of an optical diagnostic providing simultaneous temperature and composition distributions during HCCI operation.

Planar laser-induced fluorescence (PLIF) is capable of measuring two-dimensional temperature and concentration distributions with a high degree of accuracy and precision. PLIF of tracer molecules such as 3-pentanone, acetone, and toluene have seen wide spread use in IC engine research, typically for imaging of in-cylinder fuel distribution. Tracer-based PLIF measurements of in-cylinder temperature distributions have previously been demonstrated by Einecke et al. [8,9], Fujikawa et al. [10] and Kakuho et al. [11] among others. Although similar in theory, each diagnostic method varies in terms of tracer, excitation wavelengths, excitation and collection scheme, and calibration method.

In previous work by Rothamer, et al. [12-14], a two-line (i.e., dual-wavelength) PLIF technique using 3-pentanone (3P) as the fluorescent tracer was developed for simultaneous measurements of temperature and composition. The technique was optimized for in-cylinder engine conditions using available data for 3-pentanone absorption cross-section and fluorescence quantum yield (FQY) at elevated temperature and pressure [15,16]. Wavelength selection was based on a comprehensive uncertainty analysis that lead to the selection of 277nm and 308nm. Validation of this technique was performed in a motored engine under known conditions to assess measurement accuracy and precision. Additional demonstrations were also performed under fired-engine operation for both conventional HCCI and HCCI with NVO.

The present work extends the application of the two-line PLIF technique to portions of the NVO engine cycle that were previously unexplored, particularly NVO recompression and re-expansion. Both fuel-seed and air-seeded variations of the technique are applied. Fuel-seeded measurements of temperature and fuel mole fraction in the NVO recompression provide better understanding of in-cylinder conditions at the end of exhaust and early in the NVO recompression period. Similarly, measurements during NVO re-expansion help characterize gas temperatures following recompression reactions that ultimately affect main combustion phasing. Air-seeded measurements of temperature and EGR mole fraction during the main compression explore a range of NVO operating conditions, studying the effects of main and NVO injection timing on in-cylinder charge evolution. This suite of measurements is intended to address general aspects of NVO engine operation while assessing the feasibility of the diagnostic technique. The focus of this work is more on the application of the two-line PLIF technique and less about specifics of NVO engine operation. The latter topics are reserved for future publication.

BACKGROUND THEORY

The general theory and development of the two-wavelength PLIF technique have been presented in previous publications [12,13], and are replicated here as needed for clarity. The fluorescence signal in the linear regime is given by Eqn. 1,

$$S_f = \frac{E}{hc\nu} dV_c \left[\frac{x_{TR} P}{kT} \right] \sigma(\lambda, T) \phi(\lambda, T, P, x_i) \frac{\Omega}{4\pi} \eta_{opt} \quad (1)$$

where S_f is the number of photons incident [photons/pixel], E is the local laser fluence [J/cm^2], h is Planck's constant [J s], c is the speed of light in a vacuum [cm/s], ν is the laser frequency [cm^{-1}], dV_c is the probed volume [cm^3], x_{TR} is the tracer mole fraction, P is total pressure [MPa], k is the Boltzmann constant [J/K], T is temperature [K], σ is the absorption cross-section [cm^2], ϕ is the fluorescence quantum yield (FQY), Ω is the solid angle of the collection optics, and η_{opt} is the transmission efficiency of the imaging optics.

Temperature is determined by computing the ratio of fluorescence signals resulting from two excitation wavelengths. The signal ratio is given by Eqn. 2, with the calibration constant C_{cal} defined by Eqn. 3.

$$\frac{S_{f2}}{S_{f1}} = C_{cal} \frac{E_2}{E_1} \frac{\sigma_2(\lambda_2, T) \phi_2(\lambda_2, T, P, x_i)}{\sigma_1(\lambda_1, T) \phi_1(\lambda_1, T, P, x_i)} \quad (2)$$

$$C_{cal} = \frac{S_{f2}^{cal} E_1^{cal} \sigma_1(\lambda_1, T^{cal}) \phi_1(\lambda_1, T^{cal}, P^{cal}, x_i^{cal})}{S_{f1}^{cal} E_2^{cal} \sigma_2(\lambda_2, T^{cal}) \phi_2(\lambda_2, T^{cal}, P^{cal}, x_i^{cal})} \quad (3)$$

The calibration constant is determined by making PLIF measurements at homogeneous conditions of known temperature, pressure and tracer mole fraction (denoted by *cal* superscript in Eqn. 3.). These calibration measurements correct for spatial non-uniformities in laser sheet energy distribution, assuming minimal shot-to-shot variations in laser profile (sheet cross-section) and mean energy during the time between acquisition of calibration and data images. Under these assumptions the laser energy terms in Eqn. 2 and 3 will cancel.

The above equations are further simplified by defining the ratio of photophysical parameters, R_{PP} given in Eqn. 4. Substituting this relation into Eqn. 2 results in the principal equation for temperature calibration, Eqn. 5.

$$R_{PP}(T, P, x_i) = \frac{\sigma_2(\lambda_2, T) \phi_2(\lambda_2, T, P, x_i)}{\sigma_1(\lambda_1, T) \phi_1(\lambda_1, T, P, x_i)} \quad (4)$$

$$R_{PP}(T, P, x_i) = \frac{1}{C_{cal}} \frac{S_{f2}}{S_{f1}} \quad (5)$$

Performing the calibration correction in this fashion results in a measure of R_{PP} , which is itself a function of temperature, pressure and species mole fractions. The contribution of the last factor (composition) is small (but still included) in the current work due to our relatively low tracer concentrations and the modest oxygen quenching characteristics of 3-pentanone. R_{PP} is calculated as a function of these variables through knowledge of the absorption cross-section and the FQY. The absorption cross-section is calculated using curve fits developed by Koch [17]. The FQY is calculated using a ketone FQY model that is discussed in more detail in subsequent sections. Having calculated R_{PP} as a function of temperature and pressure, one can invert the function to determine temperature as a function of R_{PP} and pressure $T(R_{PP}, P)$. Finally, the calibration-corrected images determined by Eqn. 5 can be converted to temperature images.

Local composition is determined using the signal from either of the two excitation wavelengths plus the measured temperature above. The composition quantity being measured depends on where the tracer is added and how the data are processed. By seeding the fuel with tracer, we measure local *fuel* mole fraction (or concentration); by seeding both the air and the fuel, we measure the *air-plus-fuel* mole fraction. If we further assume that in-cylinder contents consist of only three quantities, intake air, fuel and EGR, we can determine *EGR* mole fraction using Eqn. 6, where x_{EGR} is the EGR mole fraction, and $x_A + x_F$ is the air-plus-fuel mole fraction.

$$x_{EGR} = 1 - (x_A + x_F) \quad (6)$$

This approach also assumes that all tracer in the air and fuel is consumed during combustion, and is not present in EGR. A similar technique was applied previously by Deshamps et al. [18] to estimate average EGR distributions, and was termed negative-PLIF due to the indirect method of measurement. The same designation is kept here, but abbreviated to N-PLIF. Both direct fuel-composition measurements and N-PLIF measurements of EGR are discussed in this work.

To calibrate mole-fraction measurements, the fluorescence signal at one excitation wavelength is divided by the corresponding calibration image described above for temperature calibration. Using this ratio to solve for x_{TR} results in Eqn. 7, where T is the measured temperature determined above.

$$\frac{x_{TR}}{x_{TR}^{cal}} = \frac{E^{cal}}{E} \frac{P^{cal}}{P} \frac{T}{T^{cal}} \frac{\sigma^{cal}(\lambda, T) \phi^{cal}(\lambda, T, P, x_i)}{\sigma(\lambda, T) \phi(\lambda, T, P, x_i)} \frac{S_f}{S_f^{cal}} \quad (7)$$

Assuming laser energy terms cancel as previously stated, all other variables in Eqn. 7 are known, and the tracer mole fraction can be calculated. For fuel-seeded measurements, the tracer and fuel mole fraction are

related by Eqn. 8, where x_S is the mole fraction of tracer seeded into the liquid fuel.

$$x_F = \frac{x_{TR}}{x_S} \quad (8)$$

For N-PLIF measurements of EGR mole fraction, the air-plus-fuel mole fraction is first determined using Eqn. 9, where, in this case, x_S is the tracer mole fraction seeded in the air and fuel, and $x_A^{cal}=1$ for motored calibration images with no fuel present.

$$\frac{x_{TR}}{x_{TR}^{cal}} = \frac{x_S (x_A + x_F)}{x_S (x_A^{cal})} = x_A + x_F \quad (9)$$

Finally, EGR mole fraction is calculated using the characteristic N-PLIF relation, Eqn. 6. Seeding the air alone does not introduce any substantial errors in EGR-fraction calculations since the fuel mole fraction constitutes an insignificant fraction of the total charge for the current NVO low-load engine experiments.

As mentioned above, an important aspect of the calibration process is calculation of the fluorescence quantum yield (FQY) using a ketone-based FQY model. This model was originally developed for acetone by Thurber [19,20], adapted for 3-pentanone by Koch [21], and later modified for engine experiments by Rothamer [12]. The exact model specifics are well documented [13], and will not be described here in detail. The model is an adapted, multi-step decay model based on excess energy of the excited vibrational states. Utilizing this frame work, model parameters are adjusted to match experimental measurements of FQY over a wide range of temperature, pressure, composition, and excitation wavelengths. The current model parameters have been adjusted to match both fundamental measurements of FQY in a heated test cell [15,22,16] and relative signal measurements made in a motored IC engine [23,12]. A benefit of this model formulation is the ability to predict FQY over a wide range of conditions, permitting accurate evaluation of potential PLIF diagnostic schemes. Laser excitation wavelength selection was based on a comprehensive measurement uncertainty analysis to optimize diagnostic performance over a range of engine conditions [12]. Based on this analysis, excitation wavelengths of 277 nm and 308 nm were selected for this work.

Table 1 : HCCI engine specifications for NVO operation

Bore	92 mm
Stroke	95.25 mm
Geometric Compr. Ratio	11.5
IVO / IVC*	-285 / -140 CAD
EVO / EVC*	140 / 285 CAD

*intake/exhaust valve open/close

EXPERIMENTAL METHODS

OPTICAL ENGINE

Measurements were performed in a single-cylinder optical engine configured for NVO experiments. The pent-roof head is a GM prototype, housing two intake valves, a single exhaust valve, and a vertical, near-centrally located 8-hole injector. The head is also equipped with two spark plug ports that have been plugged for the current HCCI experiments. The Bowditch piston is equipped with a 65-mm fused silica window, providing imaging access from below. A sample PLIF image is shown in Fig. 1 with the valves, injector and piston window superimposed in the field of view. For all PLIF images shown throughout this work, laser propagation is from image bottom to top, with exhaust and intake valves on the left and right respectively. Optical access for the laser sheets is provided by a 25-mm-tall fused silica ring incorporated into the cylinder liner. Short dwell cams (145-CAD duration) enable NVO operation, providing the high internal EGR levels required to burn high octane fuels in this engine facility. Engine specifications are provided in Table 1, with further details available in [24]. All engine measurements were performed at 1200 rpm, with iso-octane as the base fuel. Tracer was seeded in either the liquid fuel (20% 3-Pentanone by volume), or the intake air as described below. The crank angle convention used throughout this work is $-360 < \text{CAD} < 360$, with 0 crank-angle degrees (CAD) corresponding to top dead center (TDC) of main compression.

PLIF DIAGNOSTIC SYSTEM

The basic PLIF diagnostic system consists of two lasers, a Raman cell, one dual-frame ICCD camera, and associated optical components. A schematic of the PLIF diagnostic setup is presented in Fig. 2. The 308-nm laser pulse is generated by a Lambda Physik ComPexPro 102 XeCl excimer laser. The 277-nm pulse

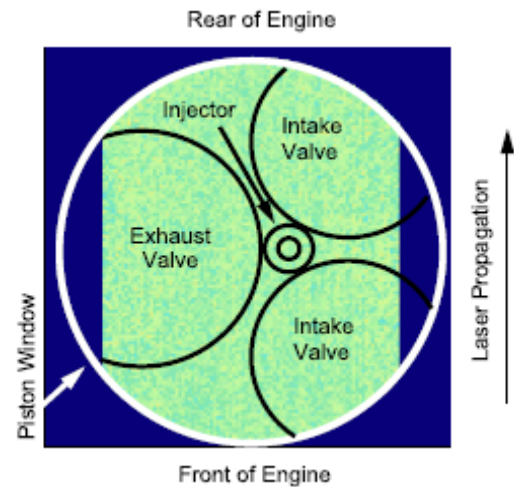


Figure 1: Sample PLIF image with valve, injector and piston window positions superimposed [13].

is generated by Raman shifting the output of a 248-nm KrF excimer laser (Lambda Physik ComPexPro 102, stable resonator) to the first Stokes wavelength (277nm) in H_2 . The Raman cell (RC) used in the current experiments (custom LightAge RC) is 72 cm in length, and is configured with a 60-cm focal length (f.l.) spherical lens at the entrance and a 40-cm f.l. spherical lens at the exit. The RC is filled with high-purity H_2 to a total pressure of 57 bar, providing approximately 10% energy conversion efficiency to the first Stokes wavelength. The output of the RC is passed through an equilateral dispersing prism to spatially separate the residual pump and shifted wavelengths, allowing the unwanted beams to be collected downstream with a beam dump.

The current setup utilizes an extended beam path length of 5-6 m for each excitation wavelength, allowing the inherent laser beam divergence to expand the beam to the desired imaging sheet dimension. Each excitation beam is passed through a 1-m f.l. cylindrical lens to form the beam waist, before being spatially overlapped on a

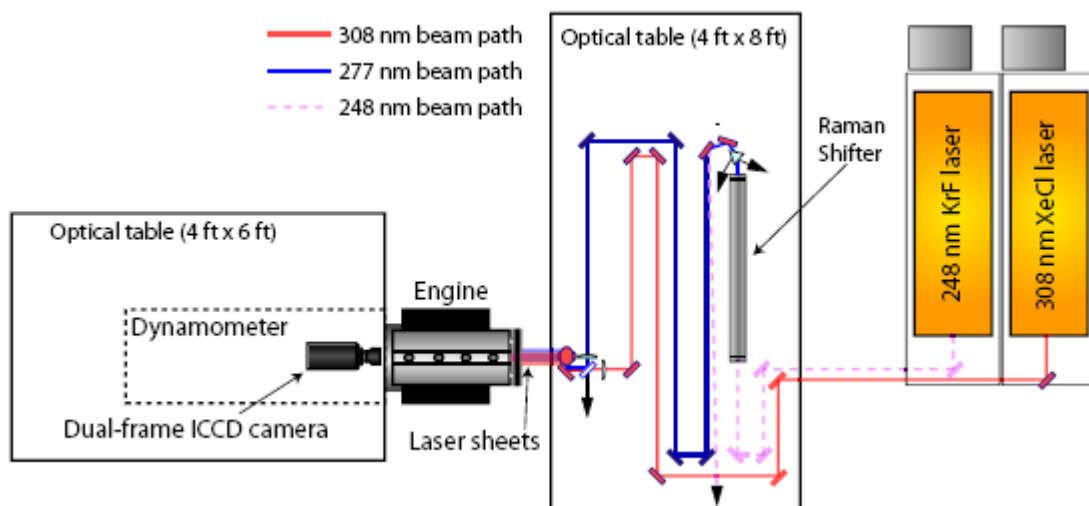


Figure 2: Schematic of experimental setup used for PLIF diagnostic [13].

dichroic element coated to reflect 277 nm and transmit 308 nm. Finally, the beams pass through a “vertical elevator” assembly that rotates the beams 90° and elevates the beam path to the desired location in the optical engine.

The resulting laser sheets are approximately 45-mm wide and 0.5-mm thick and are aligned to be parallel to the fire deck, and displaced 3 mm below. The sheets diverge slightly as they pass through the engine cylinder wall due to its effective negative focal length. Typical laser energies per pulse during experiments are 30-35 mJ for 277 nm and 45-50 mJ for 308 nm. Laser energies were measured several optical components upstream of the cylinder (before the vertical elevator assembly), and an additional 4-6% energy loss is not included in the above laser energies.

The fluorescence signal is transmitted through the fused silica piston window, and imaged onto the camera using a 85-mm f/1.4 Nikon lens. The ICCD camera (Princeton Instruments PIMAX2:1003, P46 phosphor, SB slow-gate photocathode) is equipped with an interline transfer CCD array allowing the collection of two images with inter-frame timings as low as 2 μ s. A sharp cut-on 325-nm long-pass filter is used to reject scattered 308-nm laser light. The 1024x1024-pixel CCD array is binned 8x8 on chip resulting in read-out images of 128x128 pixels (hereafter referred to as full-frame). This provides an image spatial resolution of approximately 0.5 mm, matching the out-of-plane resolution provided by the sheet thickness. In some instances the images are binned an additional 2x2 during post-processing to improve signal-to-noise ratio while sacrificing spatial resolution. For all experiments, the ICCD camera inter-frame time is set to 5 μ s, and the gate widths for the two images are set to 800 ns. The camera and laser systems are synchronized to the engine by a quarter-crank-angle-degree-resolution crankshaft encoder.

MOTORED ENGINE OPERATION

Motored engine operation is used to generate a homogeneous tracer-air mixture of known temperature, pressure and composition. Our premixed seeding system consists of a positive-displacement pump delivering tracer to a heated cell mounted on the intake air line upstream of the surge tank. The premix cell is maintained at a temperature approximately 40 K above the boiling point of the tracer to ensure rapid evaporation. The tracer flow rate is determined by measuring the mass of tracer delivered with a scale, and measuring the corresponding delivery time with a stopwatch. The air flow rate to the engine is metered with a sonic orifice. Typical seeding levels of 3-pentanone in the intake air correspond to a 3-pentanone mole fraction of between 0.1-0.3% depending on engine conditions.

The motored operating mode is used for two purposes: diagnostic validation and image calibration. For the purpose of diagnostic validation, motored experiments

are performed for a range of intake conditions, with intake temperatures ranging from 300 K to 460 K, and manifold pressures from 0.7-1.4 bar. These experiments are carried out using a “conventional” cam phasing producing approximately zero valve overlap (denoted NVO 0). Results are described in the Diagnostic Characterization section. For the purpose of image calibration, motored operation is employed between fired datasets to acquire homogeneous images required for data processing. In these experiments, cam phasing is adjusted for a valve overlap of -150 CAD (denoted NVO 150).

FIRED NVO ENGINE OPERATION

The NVO operation scheme applied in this work utilizes a dual injection strategy to achieve HCCI combustion. A representative pressure trace for fired NVO operation is shown in Fig. 3a illustrating the valve events and range of injection timings. The largest pressure peak, centered at 0 CAD, is associated with main compression and combustion, and the lesser peak, centered at +/-360 CAD, is due to NVO recompression resulting from early exhaust valve closing. Fuel injected during the NVO

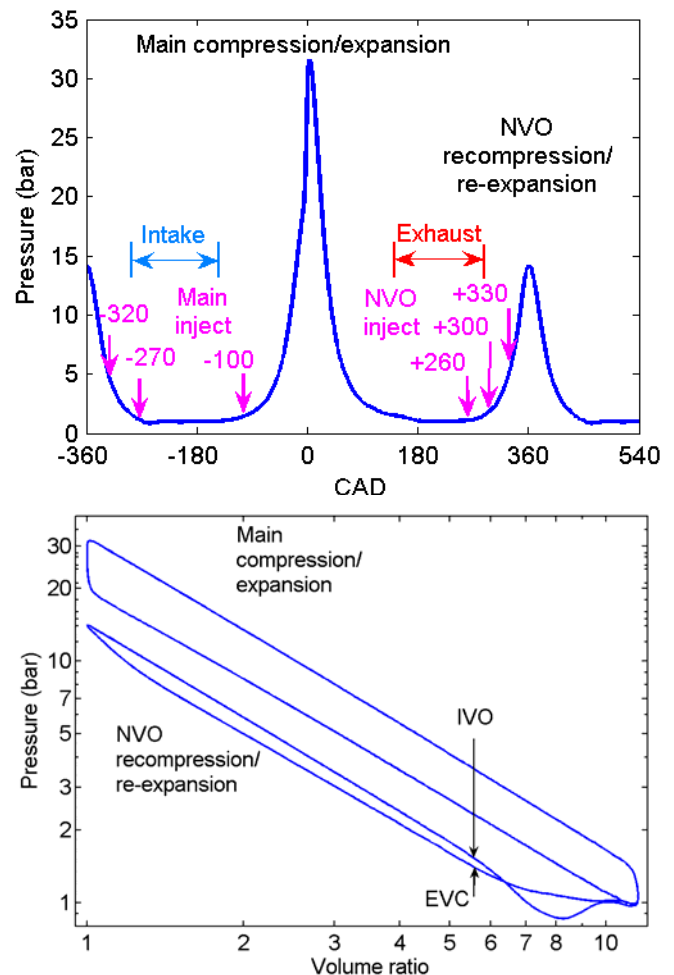


Figure 3: Measured pressure for NVO engine operation, (a) pressure vs. CAD showing valve events, injection times, and cycle nomenclature; (b) pressure vs. volume (log-log scaling).