

Effects of LIF Tracers on Combustion in a DI HCCI Engine

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ABSTRACT

Many experimental efforts to track fuel-air-residual mixture preparation in internal combustion engines have employed laser induced fluorescence (LIF) of tracers. Acetone and 3-pentanone are often chosen as tracers because of their relatively strong LIF signal, weak quenching, and reasonable match to thermo-chemical properties of common fuels such as iso-octane. However, the addition of these tracers to fuel-air mixtures could affect combustion behavior. In this work, we assess these effects to better understand limitations of tracer-based engine measurements.

The effects of tracer seeding on combustion phasing, duration, and variation are studied in an HCCI engine using a recompression strategy to accommodate single- and multi-stage-ignition fuels. Using direct-injected (DI) fuels iso-octane and n-heptane, comparisons are made of combustion performance with and without seeding of the intake air (air seeding, as opposed to the more common fuel seeding, is a variation of LIF used to measure residual-gas concentration). Chemical and premixing effects of tracer addition are distinguished by substituting equivalent amounts of fuel for the tracer. Chemical kinetic simulations of iso-octane and n-heptane oxidation help explain the experimentally determined trends.

Results show that the phasing of iso-octane combustion can be significantly impacted by premixing effects because of the sensitivity of ignition to charge temperature. For n-heptane, the chemical effects of tracer addition are shown to be more pronounced because of impact on low-temperature heat release. Acetone retards the combustion for both single- and two-stage-ignition fuels, whereas 3-pentanone advances iso-octane combustion while retarding n-heptane. Overall, we found that the impact of tracer addition is modest for the chosen operating conditions since varying the intake temperature can easily compensate for it.

INTRODUCTION

Planar laser-induced fluorescence (PLIF) of fuel tracers is used extensively to track fuel/air mixture preparation in IC engines [1-2]. By recording the fluorescence signal from two different tracers, or fluorescence from a single tracer excited by two different laser wavelengths, the diagnostic is capable of measuring simultaneous composition and temperature distributions [3-4]. In recent work [5-6], Rothamer et al. have optimized a two-wavelength PLIF technique to quantify in-cylinder distributions of residual gas fraction (RGF) and temperature in our automotive HCCI engine. In this variation of the PLIF diagnostic, both fuel and air are seeded with tracer, and RGF distribution is determined as the complement of the fluorescence signal, thereby earning the name *negative PLIF* or nPLIF [7]. An important consideration when applying such LIF diagnostics in engines is the risk of tracer addition affecting combustion performance—the current study is motivated by the need to assess this risk.

While there is abundant literature describing relevant physical and photo-physical properties of commonly used LIF tracers, there have been relatively few studies to investigate the chemical effect of tracers on combustion. Practitioners typically match important thermodynamic properties of tracers with fuels they track (e.g., boiling point and heat of vaporization), thereby increasing confidence that fuel and tracer will behave similarly through the evaporation and mixing processes. But little information is available for the subsequent combustion process. Neij, et al. [8] attempted to measure the effect of 3-pentanone addition to iso-octane and n-heptane on flame speeds in a spark-ignited engine. The experiment was inconclusive beyond a statement that any changes must be less than 20%. Zhang, et al. [9] performed similar tests and concluded that the addition of 3-pentanone or toluene to iso-octane did not negatively impact combustion performance in their spark-ignited engine.

Table 1: Fuel and Tracer Properties

Fuel/tracer	Molecular Weight [g/mol]	Boiling Point [K]	Heat of Combustion [J/mg]	Stoichiometric Fuel/Air Ratio [-]
iso-octane (IO)	114.2	372	44.4	15.1
n-heptane (NH)	100.2	371	44.5	15.1
3-pentanone (3P)	86.1	375	33.4	11.2
acetone (AC)	58.1	329	28.6	9.5

PLIF tracer concentrations are typically kept low for both diagnostic (e.g., attenuation, saturation) and engine-performance reasons. Thus for our nPLIF technique we use tracer mole fractions of about 0.2 %, but because the entire air stream is seeded, the tracer can constitute up to 15% of the total chemical energy per cycle. This large tracer fraction could have a substantial chemical effect on combustion. In addition, because the tracer is premixed with air well upstream of the cylinder, substituting tracer for direct-injected fuel is likely to have a thermodynamic premixing effect as well. The primary objective of this work is to quantify effects of tracer addition on combustion performance in order to assess the relevance of applying our PLIF measurements in conventional HCCI engines.

For this study, we have selected two fuels and two tracers. The choice of iso-octane and n-heptane as fuels allows us to examine effects of tracer seeding on both single- and two-stage-ignition fuels. For tracers, we selected acetone and 3-pentanone. They are extensively used in LIF applications for several reasons: strong signal, weak quenching, and well characterized photo-physical properties [10-13]. Table 1 provides a list of thermo-chemical properties for the fuels and tracers used in this study.

EXPERIMENTAL APPROACH

Experiments were carried out in our automotive HCCI research engine [14] configured with all-metal components to extend the range and duration of the tests. Short dwell (145 CAD) cams allow negative-valve-overlap (NVO) operation, providing the elevated RGF levels required to burn high-octane fuels such as iso-octane in our facility. The pent-roof head houses two intake valves and a single exhaust valve, as well as a vertical, centrally-located, 8-hole direct injector. The head also includes two spark plug ports, but they were plugged for these HCCI experiments. Additional engine specifications are listed in Table 2.

Table 2: HCCI Engine Specifications for NVO Operation

Bore	92 mm
Stroke	95.25 mm
Geometric Compression Ratio	11.5
Intake Valve Opening	57 CAD aTDC*
Intake Valve Closing	202 CAD aTDC
Exhaust Valve Opening	202 CAD bTDC
Exhaust Valve Closing	57 CAD bTDC

*aTDC = after top dead center

Valve event timings (Table 2) were selected to accommodate operation with both iso-octane and n-heptane fuels. The selected negative overlap measures 114 CAD, producing a residual gas fraction estimated to range from 37-46% (based on parameters determined at exhaust valve closing). This RGF is appropriate since it allows fired operation for both iso-octane and n-heptane; phasing near TDC can be achieved for both by varying intake temperature from 476 K (for iso-octane) to 333 K (for n-heptane). The coolant temperature was likewise decreased for the n-heptane tests to 333K (see Table 3).

Both premixed and direct-injected fueling are used for the experiments. Premixing is accomplished using a piston pump to meter tracer (or fuel) to a heated reservoir on the inlet air line located 1 m upstream of the intake plenum. The tracer mass flow is measured using a precision scale, the air flow rate is metered using a sonic orifice, and temperature is controlled with a series of heaters on the air lines between the sonic orifices and the engine.

Combustion performance is compared using cylinder-pressure data from a piezoelectric transducer recorded every quarter crank-angle degree and averaged over 50 engine cycles. The apparent heat-release rate is calculated from filtered pressures using conservation of energy analysis and ideal-gas assumptions presented in Ref. [15]. Combustion phasing is quantified in terms of the location of 50% of the cumulative main heat release (CA50).

The goal of quantifying effects of tracer addition was approached through the following experimental plan outlined in Tables 4 and 5. The two base fuels (identified in the top row of each table) are tested with each of three different tracers (second row of the tables): 3-pentanone, acetone, and the other fuel used as a “tracer” (i.e., iso-octane or n-heptane). For each of these tracers, we conducted a series of three tests identified in the third row of Tables 4 and 5: (i) A tracer test (abbreviated *TR*) designed to duplicate conditions of a typical nPLIF experiment, that is, the tracer is premixed in the intake

Table 3: Operating Conditions for Each Base Fuel Tested

Base Fuel:	iso-octane	n-heptane
Intake air temperature	480 K	333 K
Residual Gas Fraction	40-46%	37-39%
Coolant Temperature	363 K	333 K
Intake Manifold Pressure	100 kPa	
Fuel Injection Pressure	10 MPa	
Engine Speed	1200 RPM	

Table 4: Test Matrix for iso-Octane Base Fuel

Base fuel	iso-Octane								
Tracer	3-Pentanone			Acetone			n-Heptane		
Test abbreviation; description	TR Premix = 3P	PM Premix = IO	DI All = DI IO	TR Premix = AC	PM Premix = IO	DI All = DI IO	TR Premix = NH	PM Premix = IO	DI All = DI IO
Premix mass [mg/cycle]	2.0	1.5	0	1.35	0.8	0	2.3	2.3	0
DI mass [mg/cycle]	9.8	9.8	11.3	9.8	9.8	10.6	9.8	9.8	12.1
Intake air [mg/cycle]	336	336	336	336	336	336	337	337	337
Tracer mol% of tot. fuel	21%	–	–	21%	–	–	21%	–	–
Tracer mol% of air	0.2%	–	–	0.2%	–	–	0.2%	–	–
Intake ϕ	0.52			0.49			0.55		
HOC [J/cycle]	502			474			537		

Table 5: Test Matrix for n-Heptane Base Fuel

Base fuel	n-Heptane								
Tracer	3-Pentanone			Acetone			iso-Octane		
Test abbreviation; description	TR Premix = 3P	PM Premix = NH	DI All = DI NH	TR Premix = AC	PM Premix = NH	DI All = DI NH	TR Premix = IO	PM Premix = NH	DI All = DI NH
Premix mass [mg/cycle]	1.7	1.2	0	1.2	0.7	0	2.3	2.3	0
DI mass [mg/cycle]	7.3	7.3	8.5	7.3	7.3	8.0	7.3	7.3	9.5
Intake air [mg/cycle]	412	412	412	406	406	406	423	423	423
Tracer mol% of tot. fuel	21%	–	–	21%	–	–	21%	–	–
Tracer mol% of air	0.15%	–	–	0.15%	–	–	0.15%	–	–
Intake ϕ	0.31			0.30			0.34		
HOC [J/cycle]	380			357			423		

air, and the base fuel is direct injected; (ii) A second test repeating the first, but with the tracer replaced by an equivalent amount of premixed base fuel (abbreviated *PM*); (iii) A final test with no tracer and all the fuel direct injected (abbreviated *DI*). We selected these three tests to help sort out possible chemical and thermodynamic effects of tracer addition for our nPLIF diagnostic: comparing combustion performance from the PM and DI experiments should quantify differences due to premixing a portion of the fuel, and then comparing the TR and PM results allows an assessment of tracer chemical effects.

The second column of Table 4 (i.e., the iso-octane-base-fuel/3-pentanone-tracer/TR test) represents a test conducted at typical nPLIF experiment conditions. Parameters selected for the other tests are related to these values in the following way. The amount of premixed tracer (2.0 mg/cycle of 3P), direct-injected base fuel (9.8 mg/cycle of IO), and intake air (336 mg/cycle) represents a total intake ϕ of 0.52. For the next test in Table 4 (PM), the amount of DI fuel and the intake air are held constant, but the premixed mass becomes an equivalent amount of IO—where *equivalent amount* is defined as the mass of fuel or tracer required to keep ϕ and heat-of-combustion (HOC) values approximately constant. This approach is intended to eliminate load effects on combustion performance for each series of tests. Parameters for the third (DI) test are

the same as the PM test, except all fuel is direct injected, so ϕ and HOC again remain constant.

The same approach is applied to select parameters for the three iso-octane-base-fuel/acetone-tracer tests in Table 4. The acetone-tracer/TR test uses the same values of DI fuel and intake air as above, and the premixed mass is again adjusted to maintain approximately constant intake ϕ and HOC values. Selection of parameters for the next two (PM and DI) tests proceeds as in the last paragraph and selection of the remaining parameters in Table 4 follows similarly.

Imposing a constant seeding mole fraction (based on requirements of the nPLIF diagnostic) leads to differences in the load (HOC) for each test series (as shown in the bottom row of Table 4) due to differences in tracer heating values. Although moderate variations in combustion phasing and efficiency *between series* will result, this does not significantly impact overall conclusions about chemical and premixing effects of seeding made based on comparisons at constant load *within a series*.

To use the same valve timing for the n-heptane-base-fuel tests (Table 5) as for the iso-octane tests, we had to decrease intake air temperature substantially and reduce the total fuel load to avoid early combustion phasing. The

cooler air meant we had to increase flow to maintain a manifold pressure of 1 bar. These factors combined to reduce values of tracer/air mole ratios, intake ϕ , and HOC for the n-heptane tests. Other values in Table 5 were selected using the same approach described for Table 4.

Considerable effort was required to control operating parameters for these experiments. Combustion performance during HCCI NVO operation is very sensitive to gas and surface temperatures, and achieving steady-state operation requires long run times. In addition, we observe that the fuel-delivery rate of our DI fuel injector is sensitive to operating conditions, so that duplicating target values in Tables 4 and 5 is difficult. As a result, distinguishing the effects of tracer addition from effects of varying operating conditions is challenging. Nonetheless, the paper identifies several important qualitative trends that derive from the data.

MODELING APPROACH

To confirm and explain experimental trends observed for mixtures of fuel and tracer, CHEMKIN simulations of combustion were performed using the 0-D Closed Internal Combustion Engine Simulator by Reaction Design [16] combined with chemical kinetic mechanisms distributed by Lawrence Livermore National Laboratory [17]. Separate kinetic mechanisms for iso-octane, n-heptane, and PRF blends (i.e., mixtures of iso-octane and n-heptane) [18-20] allowed simulation of single-zone reactions and corresponding pressure profiles, heat-release rates, and species time histories.

Using temperatures, intake air amounts, residual gas fractions, and fueling amounts from the experiments, initial conditions for the model were specified at bottom dead center (BDC) of compression. The initial composition of the charge was calculated using the amount of air, fuel, and tracer introduced into the chamber plus the retained residual mass and composition, which was based on products of complete combustion in excess air. BDC charge temperature is approximated by calculating the mass-averaged temperature of the retained residuals and the intake air.

The model's heat transfer correlation was adjusted to help match simulated and experimental pressure traces. In addition, for the n-heptane base-fuel simulations, intake temperatures had to be artificially increased by about 30 K to achieve combustion phasing similar to the experiments. This adjustment stems from known difficulties phasing the characteristic low-temperature heat release (LTHR) of n-heptane during HCCI combustion [21-22]. Still, by maintaining realistic conditions and a consistent approach from test to test, the model competently predicts experimentally observed trends, offering insight into the combustion behavior of iso-octane and n-heptane.

In addition to performing 0-D engine simulations, CHEMKIN was also used to simulate ignition delay times for the base fuels and tracers of interest in this study. Ignition delays for each were determined for stoichiometric conditions, constant pressure of 12 atm, and for temperatures ranging from 900 to 1400K. The same simulations were also carried out over a range of pressures in order to validate the model with available shock tube ignition time measurements for each of the constituents.

EXPERIMENTAL AND COMPUTATIONAL RESULTS

EFFECT OF FUEL PREMIXING IN THE INTAKE PLENUM

Before looking at the chemical effect of seeding the intake air with tracer, it is helpful to establish the effect of premixing a portion of the fuel in the intake air plenum (PM) rather than mixing all of it in the cylinder via direct injection (DI). Because three different load levels of base fuel are needed to maintain the HOC for each comparison. Indicated mean effective pressure (IMEP) and combustion phasing (CA50) of the DI and PM tests for each load level of iso-octane are shown in Figure 1 to illustrate the effect of premixing on combustion. Results for 50 consecutive cycles are plotted along with calculated mean values for each test and calculated coefficients of variation (COV) of IMEP.

At the highest iso-octane fuel load (12.1 mg), there is a clear separation of the CA50 data between the DI and PM tests, showing that premixing 2.3 mg of the fuel in the intake air plenum has the effect of advancing CA50 by nearly 2 CAD on average. Similar trends were observed to a lesser degree for the lower load cases of 11.3 and 10.6 mg of iso-octane; the degree of

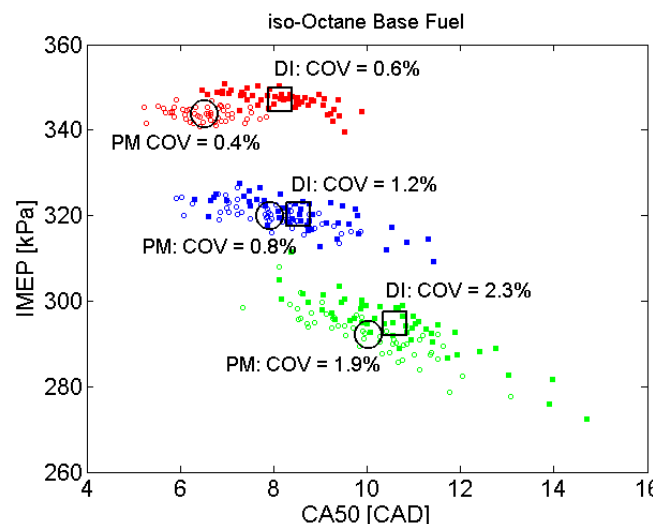


Figure 1. Effect of premixing on iso-octane combustion phasing at three different loads for DI (filled squares) and PM (open circles) tests. Six large symbols represent cycle-averaged values.