

# The Combined Effect of HCHO and C<sub>2</sub>H<sub>4</sub> Addition on Combustion in an Optically Accessible Diesel Engine Fueled with JP-8

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Marcis Jansons, Radu Florea, Kan Zha and Elena Florea  
Wayne State University

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## ABSTRACT

Misfiring or partial combustion during diesel engine operation results in the production of partial oxidation products such as ethylene (C<sub>2</sub>H<sub>4</sub>), carbon monoxide and aldehydes, in particular formaldehyde (HCHO). These compounds remain in the cylinder as residual gases to participate in the following engine cycle. Carbon monoxide and formaldehyde have been shown to exhibit a dual nature, retarding ignition in one temperature regime, yet decreasing ignition delay periods of hydrocarbon mixtures as temperatures exceed 1000 °K. Largely unknown is the synergistic effects of such species. In this work, varying amounts of C<sub>2</sub>H<sub>4</sub> and HCHO are added to the intake air of a naturally-aspirated optical diesel engine and their combined effect on autoignition and subsequent combustion is examined. To observe the effect of these dopants on the low-temperature heat release (LTHR), ultraviolet chemiluminescent images are recorded using intensified CCD cameras. High-speed, crank-angle resolved visible range images are recorded to examine soot-forming tendencies in the latter stages of combustion. Chemical kinetics modeling using a detailed hydrocarbon mechanism and a JP-8 surrogate blend is applied to track the behavior of HCHO, C<sub>2</sub>H<sub>4</sub>, OH, pyrene and HCHO\*-producing reactions throughout the autoignition process. HCHO, in concentrations that may realistically be found to result from a partially firing or misfired engine cycle, is shown to effectively retard LTHR, increase ignition delay, and decrease the peak magnitude of the ARHR in a diesel engine operated with JP-8 under light load conditions. Further, this compound is found to suppress HCHO\* chemiluminescence and act as an effective soot-promoter. Ethylene, C<sub>2</sub>H<sub>4</sub>, alone was not observed to influence LTHR or ignition delay, however, did marginally

increase observed visible soot emission. Results identify formaldehyde as a species whose role and kinetic effects should be considered during diesel engine starting.

## INTRODUCTION

Factors influencing autoignition of fuel-air mixtures include temperature, density, induction duration and composition. The ignition delays of such mixtures have classically been described by Arrhenius-form fits of empirical data over a limited range of engine types and conditions [1,2]. The kinetic effects of minor species present as a result of varying degrees of oxidation, or as residual, have been recognized, if not fully understood, and implemented through fuel preconditioning techniques such as fumigation and pilot injection [3].

The determination of the role of combustion intermediates plays a role in several practical applications. In the quest for achieving simultaneous low nitrogen oxide (NO<sub>x</sub>), and low particulate matter (PM) engine-out emissions, the concept of homogeneous charge compression ignition (HCCI) has been advanced [4,5]. Among the current obstacles preventing the application of this combustion mode to practical systems is the lack of an effective means to control the kinetic oxidation process upon valve closing. As a possible solution, the kinetic-modifying effects of adding re-circulated exhaust gas (EGR) have been examined [6,7]. The 913 species found in a detailed hydrocarbon mechanism have more specifically been ranked by Aceves *et al* [8] by their effect in advancing combustion in HCCI combustion.

Kinetically altered autoignition is also an important issue during the cold-starting of diesel engines. Marginal autoignition conditions result from low temperatures, and

associated reduced fuel evaporation rates and fuel wall impingement. Particularly, when charge temperatures are below 1000K, secondary variables other than temperature and pressure play deterministic roles in the ignition delay [1]. EGR has been applied as an aid in diesel engine cold-starting, although the relative contribution of the kinetic and thermal effects is not fully understood [9].

Combustion instabilities have been observed during the cold-start of diesel engines, resulting in elevated fluctuations of either indicated mean effective pressure (IMEP) or engine speed [10,11]. Earlier work in this laboratory has observed fluctuations in ultraviolet (UV) chemiluminescence during the compression stroke, prior to fuel injection, during such an unsteady sequence of engine cycles during a cold-start [12]. During this sequence, a high degree of correlation was shown between this pre-injection chemiluminescence, and the combustion phasing of the following cycle, with a high UV signal predicting advanced combustion following the injection event. Spectral analyses suggested that the source of chemiluminescence emission is formaldehyde (HCHO), which was also found in the exhaust gas analysis.

HCHO has been found to inhibit hexane combustion in a reaction chamber [13], and retard ignition delay in a diesel engine operated both in a conventional mode with diesel fuel, and with methane and propane fuels ignited with a diesel pilot injection [14]. In HCCI experiments using blends of n-butane and methane, Furutani determined that HCHO addition advanced ignition of fuel blends having higher methane fractions, but retarded those more heavily weighted with n-butane, suggesting the HCHO interaction depends on fuel type [15]. A subsequent work has shown that HCHO advances ignition at temperatures above 900K, but retards ignition below this value due to OH scavenging effects [16]. Of interest in this work is the observation that HCHO addition below 900K eliminates OH radical light emission. The ignition-retarding effect of HCHO has been supported by Konno in other work using di-methyl ether (DME) fuel [17]. In addition to HCHO retarding HCCI ignition, a reduction in total heat release has been reported [18]. Experiments in this laboratory have similarly documented an autoignition-inhibiting, heat-release depressing effect of HCHO in a conventional diesel engine operated with jet propulsion fuel JP-8. Additionally, the addition of HCHO to the engine inlet was found to suppress broadband UV chemiluminescence, and to dramatically increase yellow-orange combustion luminosity [19]. Thus, the literature suggests that HCHO plays an important, but complicated role in both diesel and HCCI autoignition, depending on temperature and fuel types.

To illustrate the variability of residual composition during a diesel engine cold-start, a compression and expansion process was examined using an adiabatic HCCI model having a compression ratio of 15. In this model, the oxidation process of a homogeneous lean ( $\Phi=0.1$ ) mixture of a JP-8 surrogate

initially at 300K and 1 bar pressure was followed over a range of engine speeds. The surrogate blend chosen has been described by Violi *et al* [20], and includes aromatic as well as straight, branched, and cyclic paraffins in the proportions shown in Table 1. The hydrocarbon kinetic mechanism by Ranzi *et al*, [21] and this particular surrogate have been found to most closely predict ignition delays measured in shock tube experiments [22], and both have been used here. This mechanism contains 380 species, C1-C16, in 11,112 reactions.

**Table 1. JP-8 Surrogate used for kinetic modeling (Violi *et al* [20]).**

| Component | Component Name      | Composition (%) |
|-----------|---------------------|-----------------|
| IC8H18    | Iso-octane          | 5.5%            |
| C6H6      | Benzene             | 1%              |
| C7H8      | Toluene             | 10%             |
| MCYC6     | Methyl Cyclo-hexane | 10%             |
| NC12H26   | Dodecane            | 73.5%           |

The rationale for this model is that copious fuel wall impingement during diesel engine cold-start results in continuous fuel evaporation during all four engine strokes, including intake and compression. Resulting conditions are expected to be lean and well-mixed due to the large amount of time available. The degree of oxidation this mixture undergoes is dependent upon the cyclic temperature-pressure history experienced by a particular engine cycle.

The composition at the end of the modeled compression and expansion strokes is shown in Figure 1. At sufficiently reduced speeds, the oxidation process tends more towards completion, as evident by the mole fraction of carbon dioxide (CO<sub>2</sub>). At very high engine speeds, insufficient time is allowed for the kinetics process, and the composition after expansion is largely similar to that prior to compression. In between, however, is a range of engine speeds where intermediate species are created in appreciable amounts and subsequently frozen. These species include carbon monoxide (CO), hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>), and hydrogen (H<sub>2</sub>), in addition to HCHO and ethylene (C<sub>2</sub>H<sub>4</sub>). Charge composition into which fuel is injected then may be expected to vary accordingly.

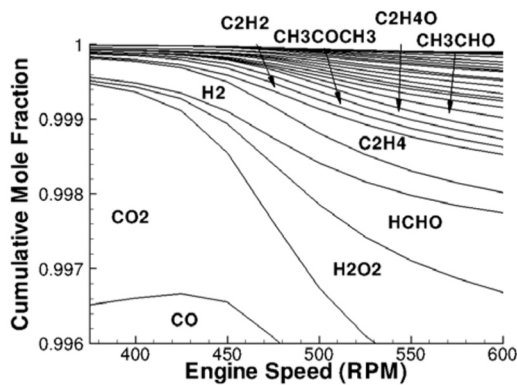


**Figure 1. Modeled cumulative mole fractions of mixture at end of expansion cycle of adiabatic HCCI process. Composition of partial oxidation products varies greatly with engine speed. Equivalence ratio = 0.1, initial temperature=300K, initial pressure=1 atm, compression ratio=15. Violi JP-8 surrogate [20] and Ranzi kinetic mechanism [21].**

Examination of [Figure 1](#) reveals that not only do the mole fractions of the intermediate species vary, but so do their relative proportions. Thus, if two intermediate species have different degrees of influence over retarding combustion, their combined influence may be expected to greatly vary over a range of over several hundred RPMs, as experienced during an engine start. [Figure 2](#) shows the ratios between HCHO, C2H4 and H2O2 fractions. Under the modeled conditions, of the three ratios, the fraction of HCHO to C2H4 varies most, from a value over ten at 200 RPM, then declining with engine speed to remain relatively unchanged at 2.5 from 550 RPM to the highest speed examined, 1800 RPM.

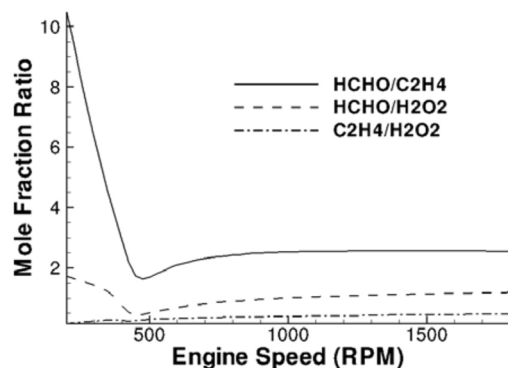


**Figure 2. Modeled ratios of C2H4, HCHO and H2O2 in cylinder gases at end of expansion stroke of adiabatic HCCI process. HCHO/C2H4 Ratio varies greatly with engine speed. Equivalence ratio = 0.1, initial temperature=300K, initial pressure=1 atm, compression ratio=15. Violi JP-8 surrogate[20] and Ranzi kinetic mechanism [21]**

This work describes an experimental investigation of the effects of HCHO and C2H4 on combustion in an optical diesel engine that is fueled with JP-8 and operated under light load conditions. Controlled amounts of these compounds are introduced to the engine intake, and ultraviolet chemiluminescence and high-speed luminous images of autoignition and the subsequent combustion process are recorded. Detailed kinetic modeling is pursued in an attempt to explain the experimental observations.

While the kinetic role of residual gases on autoignition has long been recognized, relatively little attention has been paid to identifying and understanding the role of the individual half-dozen or so “major” components of residual gases. This work attempts to illustrate the effect of two such species, C2H4 and HCHO, in a conventional diesel engine. There is a clear application to cold-starting, where an engine control unit may optimally compensate injection timing in response to the particular speed or conditions where a misfire is detected. The autoignition-modifying role of HCHO in particular is also applicable to several kinetically-controlled combustion concepts that are currently under development. These include Partially Premixed Combustion (PPC) [23], fuel-reactivity controlled Premixed Charge Compression Ignition (PCCI) engines [24] and HCCI controlled through negative-valve overlap fuel injection [7]. Moreover, residual effects may not be negligible when premixed combustion is employed to obtain high-temperature, high-pressure conditions for ignition studies.

## EXPERIMENTAL SETUP

### ENGINE

The engine used in this investigation is a naturally-aspirated, single-cylinder, direct-injection AVL Model 5402 optical-access research engine with a bore of 85 mm, stroke 90 mm and resulting displacement of 510 cm<sup>3</sup>. The geometric compression ratio has been measured to be 15:1. The intake ports are equipped with a swirl control valve, allowing the control of swirl ratios between 2.0 and 4.5. This engine is equipped with a Bosch CR CP1 common-rail fuel injection system rated to 1350 bar injection pressures. Engine and injection system specifications are shown in [Tables A1 and A2](#) of the [Appendix](#).

Optical access is provided via a classic Bowditch extended piston in which is mounted a 20 mm-thick sapphire window, as shown in [Figure 3](#). The placement of a mirror inside the piston assembly at 45° relative to the cylinder axis provides a view of the entire 40 mm-diameter combustion bowl. The combustion bowl is of rectangular cross-section, and the flat surface geometry of the combustion chamber is interrupted only by valve pockets placed in the piston bowl rim and valve seat chamfers in the cylinder head. Oil-less lubrication is provided by slotted graphite rings and the sealing by

uninterrupted bronze-Teflon rings. Compressed air directed at the underside of the piston window provides cooling of this assembly during operation.

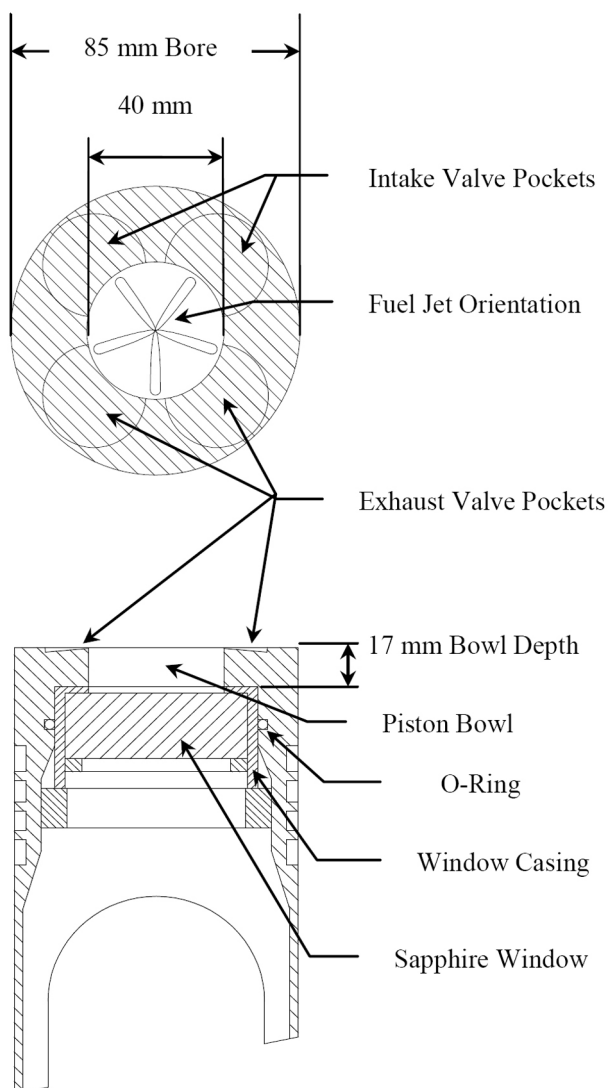


**Figure 3. Extended piston and combustion bowl geometry.**

## ENGINE INSTRUMENTATION

To measure cylinder pressures, an un-cooled piezo-electric pressure transducer (AVL GH 12 D) is mounted through an opening in the cylinder head. A needle lift sensor (MicroEpsilon) is installed in the fuel injector to detect the displacement of the injector needle. An additional pressure transducer measures the pressure in the line between the fuel rail and injector. Sensor signals are recorded by a high-speed data acquisition system triggered by an optical encoder wheel mounted on the engine crankshaft. This instrumentation is used to calculate the Apparent Rate of Heat Release (ARHR) using the analysis provided by Heywood [1], and is shown normalized by the engine displacement. A more detailed

description about the engine and instrumentation has been reported earlier [25].

Chemiluminescent images of the combustion chamber were captured through the piston window using an intensified charge-coupled device camera (ICCD), (Princeton Instruments PI-MAX3) whose GENIII intensifier has a nominal sensitivity spanning the range from 175 to 870 nm. This range effectively covers the chemiluminescence spectrum of species such as HCHO, OH, CH, C<sub>2</sub> and CO<sub>2</sub> [26] that occurs in the early stages of diesel autoignition [27], as well as the yellow-orange thermal soot emission. A visible range color camera (Vision Research Phantom 7.3) was used to obtain high speed cycle-resolved images. Frames were triggered at 0.5 CAD intervals and synchronized to the crankshaft position through a field-programmable gate array (National Instruments) and optical-encoder compatible input module (DRIVEN).

Figure 4 shows the experimental layout with the ICCD aligned with the axis of the extended piston through the 45° mirror. In such a configuration, the camera field of view, as represented by the circle in Figure 5, covers the 40 mm-diameter combustion bowl. Swirl motion is in the clockwise direction.

Formaldehyde in an aqueous solution of 37% (vol/vol), was kept in a stainless steel vessel that was pressurized by nitrogen to a value of 30 psi. A commercial port-fuel injector was then electronically controlled to meter the solution into the throat of an atomizing venturi, which was connected to a supply of dry, compressed air. The outlet of this venturi delivered the spray into a 50-gallon mixing drum, which doubled as a surge tank and had a second inlet that was open to the ambient pressure of the laboratory. Gaseous C<sub>2</sub>H<sub>4</sub> from a pressurized bottle was also introduced to the mixing tank, with the delivered amount controlled by a pressure regulator and flow control valve. The amounts of C<sub>2</sub>H<sub>4</sub> and HCHO thus added were continually monitored by a Fourier Transform Infrared spectrometer (FTIR) [28,29]. After optimizing the HCHO injection pulse duration and injection pressure, and the C<sub>2</sub>H<sub>4</sub> pressure regulator and control valve settings, a reasonable degree of control over the mole fraction of the dopants in the intake air could be achieved. Moreover, by adjusting the flow rate of the dry, compressed air running through the atomizing venturi, humidity levels in the engine inlet could be controlled independently of the HCHO, as the moisture-free compressed air could compensate for the water injected along with the HCHO.

## ENGINE OPERATING CONDITIONS

Experimental results reported here are taken from the optical engine that had been pre heated to a temperature of 60 °C. In a typical experimental sequence, the engine was motored while C<sub>2</sub>H<sub>4</sub> flow rates and HCHO solution injection duration

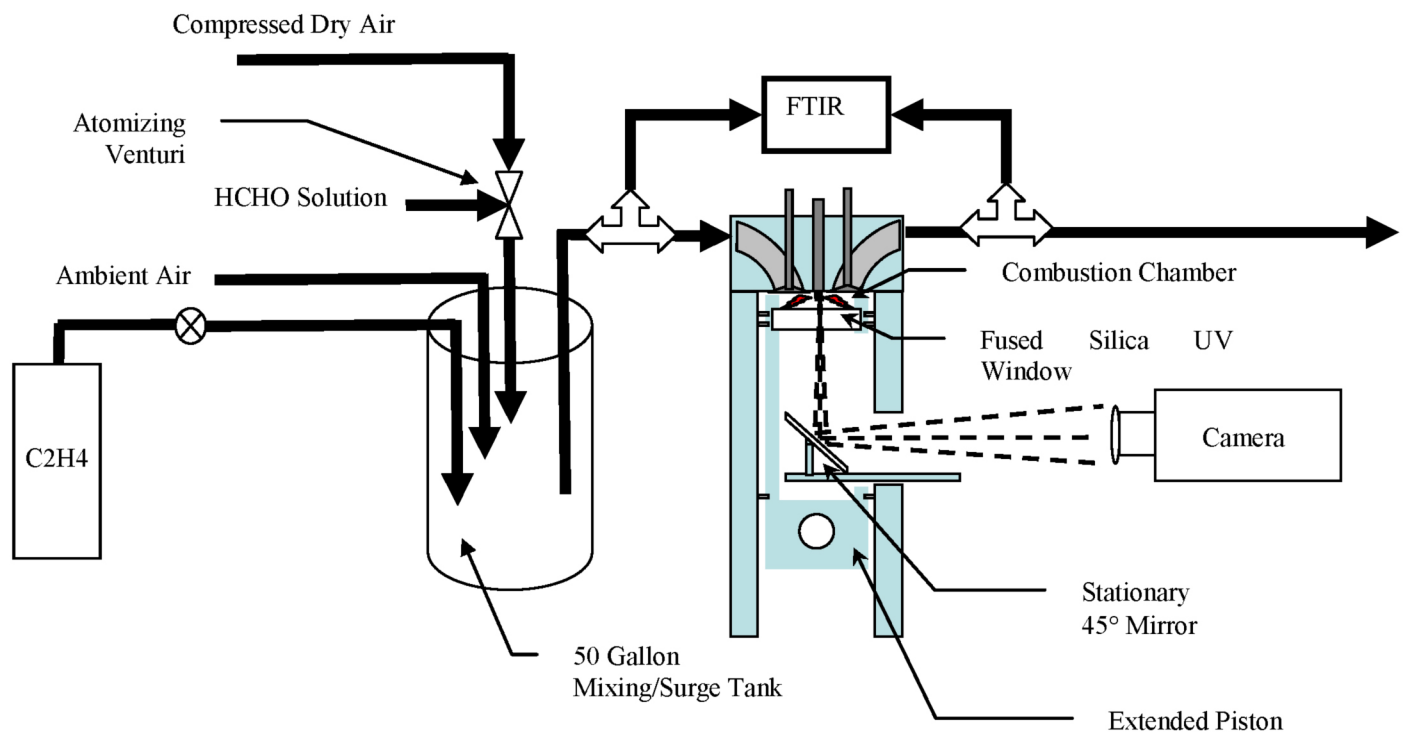


**Figure 4. Experimental setup, optical access via Bowditch piston, C<sub>2</sub>H<sub>4</sub> and HCHO metering system.**

and compressed air flow rates were adjusted to achieve steady, desired ethylene, formaldehyde and water vapor concentrations. The engine was then continually fired to warm up surfaces to values more closely resembling engine operating conditions. In an attempt to control for varying degrees of cylinder sealing by the oil-less rings, the cylinder pressure prior to fuel injection was monitored. When a predetermined value was reached, engine operation was switched to a 3/9 injection/skip pattern. The engine was operated in skip mode until the cylinder pressure prior to fuel injection was deemed steady, and then data collection was begun. The work reported here consists of measurements taken from the engine operated at speed of 1200 RPM at a swirl ratio of 2.0. For all experiments, the fuel was administered in a single injection at an injection pressure of 800 bar. The injector command signal was constant at 430  $\mu$ sec, corresponding to an estimated fuel delivery rate of 6 mm<sup>3</sup>/cycle (4.8mg/cycle). Only the third firing cycles of each sequence are considered in the ARHR calculations presented, as the third firing cycle is believed to more closely represent operating engine conditions in terms of surface temperatures and residual composition. Inlet temperatures and pressures were at ambient levels.

## FUEL

Jet Propulsion fuel (JP-8) was used during experiments. The atmospheric pressure distillation curve of this fuel, as provided by the supplier, is shown in Figure 6. JP-8 fuel is used by the US Military for powering both gas turbine and

reciprocating powerplants, and was chosen to further characterize its performance in the latter type of engine. Noteworthy features of this fuel are its low aromatic content (14% by volume) and a 50% distillation point of 206 °C, a temperature that is nearly 50 °C lower than for ultra-low sulfur diesel (ULSD) fuel typically used in this laboratory. This fuel can then be considered more volatile and with less soot-forming tendency than ULSD.

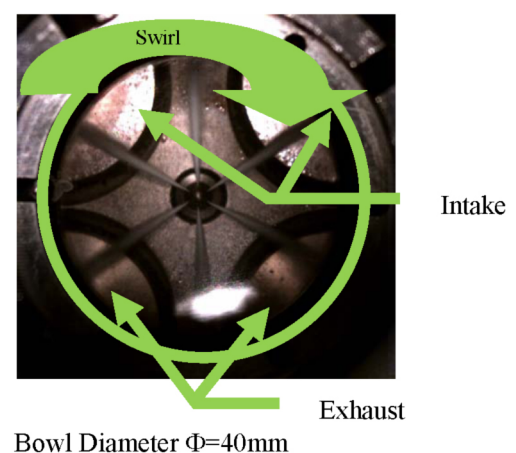


**Figure 5. Camera field of view relative to combustion chamber, swirl direction (clockwise) and spray orientation.**

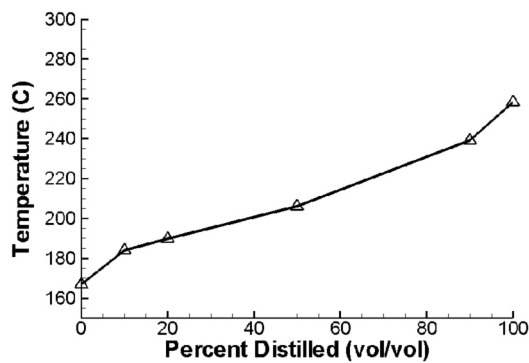


Figure 6. Atmospheric pressure distillation curve for JP-8 fuel used during experiments.

## EXPERIMENTAL RESULTS

To verify the modeled predictions of variation in intermediate species concentrations with temperature-pressure history, the engine was operated to intentionally misfire through retarded start of injection while an exhaust gas analysis was performed with an FTIR instrument. This experiment is not an attempt to quantitatively replicate the results of Figure 1, but rather to qualitatively validate the change in composition with varying temperature-pressure history. The average cycle pressures and ARHR of each sequence of cycles operated under the three conditions examined are shown in Figure 7. At a fuel delivery of  $6\text{ mm}^3$  per cycle ( $4.8\text{ mg/cycle}$ ) at a Start of Injection (SOI) of  $3^\circ$  bTDC produced a partially misfiring condition exhibiting late combustion. The injection was then further retarded, to an SOI of  $0.5^\circ$  bTDC, while maintaining the  $6\text{ mm}^3$  per cycle fueling rate. Lastly, the SOI was maintained at  $0.5^\circ$  bTDC, and the fueling rate increased to  $9.2\text{ mm}^3$  ( $7.4\text{ mg/cycle}$ ). The mole fractions of five species as measured by the FTIR in the engine exhaust are shown in Table 2, along with the standard deviation of this value over the time interval of the measurement. CO mole fraction decreased in the completely misfiring cases, as temperatures are insufficiently high for its significant formation. On the other hand, ethane ( $\text{C}_2\text{H}_6$ ) and methane ( $\text{CH}_4$ ) mole fractions show an order of magnitude increase between the same conditions. HCHO and  $\text{C}_2\text{H}_4$  levels remain steady over the three conditions on the order of 200 ppm and 25 ppm, respectively. With the exception of  $\text{C}_2\text{H}_4$ , the mole fractions measured were of the order of those predicted by the HCCI model above. Local in-cylinder mole fractions in the vicinity of the fuel jets are expected to be even greater.

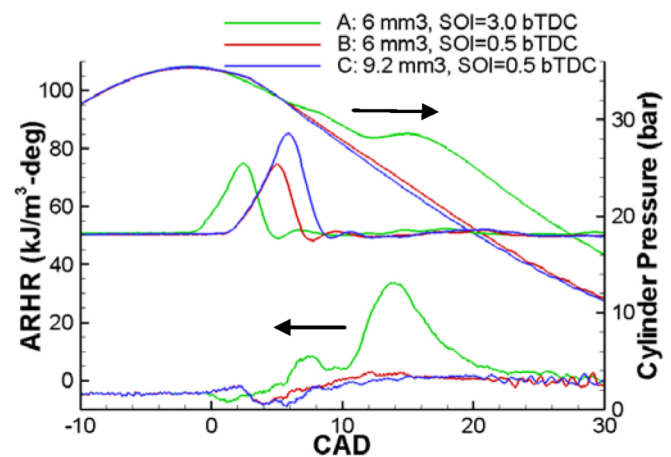


Figure 7. Average cylinder pressure, ARHR and Needle Lift signal (in arbitrary units, not shown) of partially firing and misfiring cycles yielding FTIR exhaust gas analyses shown in Table 2. Engine speed=1200 RPM, fuel delivery quantities and Start of Injection as shown.

Broadband UV chemiluminescent images were taken through the low temperature heat release (LTHR) period of the autoignition process at various levels of HCHO and  $\text{C}_2\text{H}_4$  intake doping between 0 and 1000 ppm. The ARHR plots from five combinations are presented in Figure 8, followed by the images in Figure 9. Since the ICCD camera used for these images can only record a single image per engine cycle, and multiple 'accumulations' are used for each frame, the sequence shown is a composite recorded over many cycles. Exposure times were  $70\mu\text{sec}$ . The ARHR bold plot is the average for each crank angle recorded over all the cycles used for the images, with the traces of the individual cycles shown in light gray to illustrate the degree of experimental variability.

From the baseline case without any dopant, in black, the addition of 1000 ppm  $\text{C}_2\text{H}_4$ , in blue, has an imperceptible effect on the LTHR. No effect on HTHR ignition delay is evident. The peak ARHR, at a value near  $90\text{ kJ/m}^3$  per degree, however, is greater due to the added energetic value of the  $\text{C}_2\text{H}_4$ , which is retarded by a fraction of a degree. To the contrary, the 1000 ppm HCHO addition slightly diminishes the magnitude of the LTHR, the peak of which is retarded by nearly a full crank angle degree, as is the HTHR ignition delay. The addition of 1000 ppm HCHO reduces the peak ARHR to  $60\text{ kJ/m}^3$  per degree; however the kinetic effect of HCHO here is compounded by the increased ignition delay pushing the HTHR further into the expansion cycle. While a further addition of 1000 ppm  $\text{C}_2\text{H}_4$  has no detectable effect on the LTHR or ignition delay, it does however increase the peak ARHR by nearly  $10\text{ kJ/m}^3$  per degree. The addition of 600 ppm HCHO and 500 ppm  $\text{C}_2\text{H}_4$  results in an ARHR trace evenly between the extremes. These results clearly show that ethylene,  $\text{C}_2\text{H}_4$ , has a marginal