

A Fuel Surrogate Validation Approach Using a JP-8 Fueled Optically Accessible Compression Ignition Engine

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ABSTRACT

An experimental fuel surrogate validation approach is proposed for a compression ignition application, and applied to validate a Jet-A POSF 4658 fuel surrogate. The approach examines the agreement of both physical and chemical properties of surrogate and target fuels during validation within a real compression-ignition engine environment during four sequential but distinct combustion phases. In-cylinder Mie Scattering measurements are applied to evaporating sprays to compare the behavior of the surrogate, its target fuel, and for reference, n-heptane. Early mixture formation and low temperature reaction behavior were investigated using 2-D broadband chemiluminescence imaging, while high temperature ignition and combustion chemistry were studied using OH chemiluminescence imaging. The optical measurements were combined with cylinder pressure-based combustion analysis, including ignition delay and premixed burn duration, to validate the global behavior of the surrogate. Engine-out UHC, NO and soot emissions were also compared at different intake conditions, injection pressures and injection strategies. The proposed approach can provide validation data for further numerical engine combustion modeling and kinetic mechanism validation.

The results show the surrogate was able to match the spray behavior, high temperature radical distribution, high temperature ignition delay, and the premixed burn duration of the target Jet-A fuel. Reasonable agreement was observed between low temperature ignition delay and radical distribution. The surrogate also captures the trend of the effects of intake conditions and injection pressure when single or double injections are used.

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INTRODUCTION

Engine development and combustion optimization costs can be greatly reduced through the use simulation tools. Since the auto-ignition process in a compression ignition engine is primarily driven by chemical kinetics [1], detailed fuel chemistry is required to enable predictive combustion and emissions modeling. However, the prohibitive computational expense and lack of kinetic data preclude consideration of all of the species found in a common distillate fuel, the number of which can reach into the hundreds. Hence, fuel surrogates, comprising mixtures formed from a limited number of pure compounds, are chosen to represent the physical and chemical kinetic behavior of a real fuel. A key element to surrogate development is the validation required to establish the fidelity of the emulation of the target fuel within a practical combustion system.

The U.S. military's Single Fuel Concept mandates the compatibility of all military combustion devices with jet fuel, including conventional compression ignition diesel engines. Current jet fuels can be derived from a variety of alternative sources, and possess a wide range of physical and chemical properties [2, 3], including

autoignition tendency. The formulation of jet fuel surrogates may therefore differ depending on the selected target properties [4,5,6,7,8,9]. The importance of the target properties is also application dependent. For example, a surrogate developed for a turbine application may not consider autoignition tendency as a target property, which for a reciprocating engines is paramount. Fundamental shock tube, flow reactor and rapid compression machine experiments [10,11,12,13,14,15,16,17,18] are often used to validate JP-8 surrogate gas phase ignition delays. However, many practical combustion devices have unique operating conditions involving different physical and chemical processes. A fuel surrogate designed to reproduce the behavior of a target fuel in one combustion system may not do so in another [19]. For example, a fuel surrogate validated with fundamental gas phase constant volume or flow reactor ignition experiments may fail to capture physical phenomena important to mixture formation processes that lead to ignition within compression ignition engines, such as spray breakup and evaporation. In addition, the internal combustion engine operates under varying temperature and pressure time histories which require the surrogate to be examined in multiple ignition regimes: low, intermediate and high

temperature) within a single cycle. Therefore, engine experiments are required to further validate the jet fuel surrogate within real environments [20, 21].

In this work, a systemic approach is proposed for validating a Jet-A (POSF 4658) surrogate within an optically-accessible compression ignition engine with varying intake conditions and injection pressures with both single and double injections. The use of the optical engine allows the application of optical diagnostic techniques to provide spatial and temporal insights into the spray and kinetic processes during surrogate validation. Figure 1 shows the surrogate validation approach which examines four sequential processes occurring within the combustion chamber beginning from the start of fuel injection. First, evaporating spray liquid penetration measurements are made to compare the in-cylinder spray behavior of the surrogate to its target fuel. Secondly, low temperature 2-D chemiluminescence imaging is used to verify similar intermediate radical distribution during the low temperature heat release period. Thirdly, the auto-ignition radical distribution is validated using OH chemiluminescence imaging.

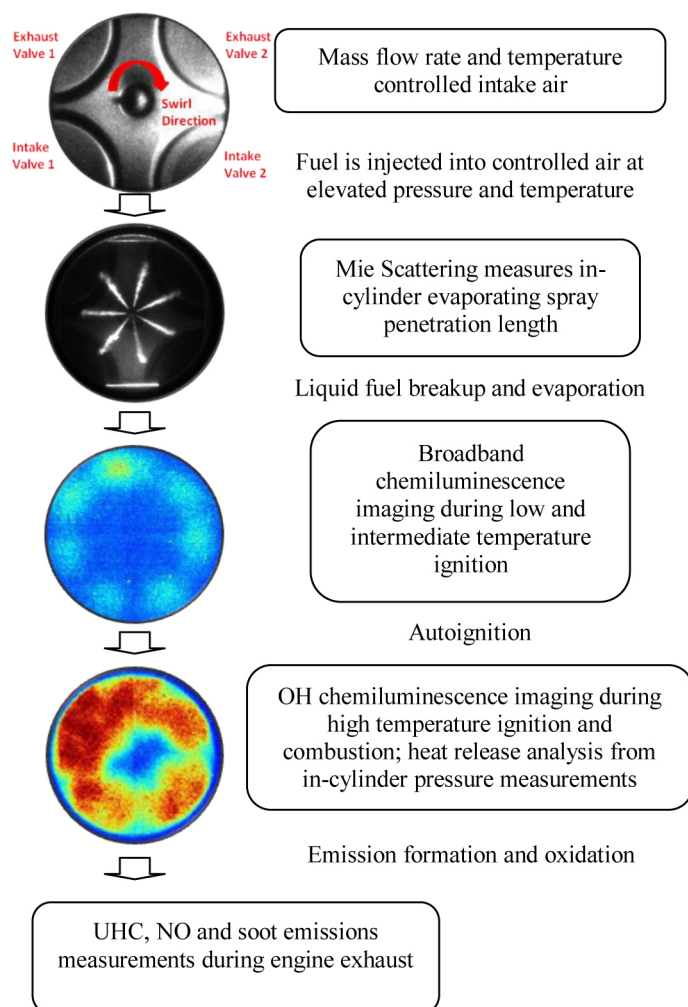


Figure 1. Steps of the experimental surrogate validation approach.

Finally, conventional cylinder pressure-based global heat release analysis and engine-out emissions are compared for the surrogate and target fuel as metrics of the overall oxidation process. These data can be further used for CFD model validation, providing 2-D measurements that can be spatially compared with reacting 3-D CFD predictions with the surrogate.

EXPERIMENTAL SETUP AND METHODS

Engine Configuration and Instrumentation

The experiments were performed in a single-cylinder, direct injection optically accessible research engine (AVL Model 5402) with a custom designed intake system that uses a sonic nozzle to regulate the air mass flow rate, an electric heater with a feedback controlled circuit to maintain the intake air temperature, and an insulated surge tank to reduce intake pressure pulsations. Figure 2 shows the configuration which allows the intake temperature to vary while keeping the same engine intake air density and *vice versa*.

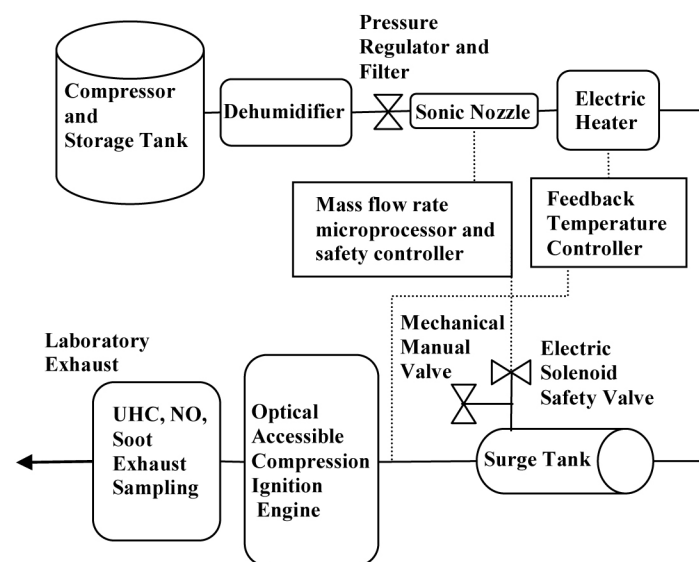


Figure 2. Schematic of the intake, engine and exhaust sampling system.

The cylinder pressure was measured by an un-cooled piezo-electric pressure transducer (AVL GH 12 D) mounted in the cylinder head. Another strain gauge pressure transducer (AVL SL31D-2000) was used to measure the pressure of the fuel line between the common rail and the injector. A current probe was attached to the injector wire to detect the current profile controlling the injection process. These sensor signals were recorded by a high-speed data acquisition system (AVL IndiCom) triggered at 0.1 CAD intervals and synchronized to engine position by an optical encoder wheel mounted on the crankshaft. The high-resolution pressure data obtained from the system was used to calculate the Apparent Rate of Heat Release (ARHR) according to the analysis provided by Heywood [22], and normalized by the engine displacement. The engine geometry is shown in Table 1 while the injector configuration is shown in Table 2. A more detailed description of the engine and instrumentation has been reported earlier [23,24,25,26].

Table 1. Engine geometry configuration

Engine Type	AVL 5402, DI
Number of Cylinders	1
Cycle	4-stroke
Displacement	510 cm ³
Bore	85 mm
Stroke	90 mm
Connecting Rod Length	148 mm
Geometric Compression Ratio	15:1
Combustion Bowl Diameter	40 mm
Combustion Bowl Depth	14.5 mm
Number of Intake Valves	2
Number of Exhaust Valve	2
Intake Valve Opening/Closing	294° aTDC/154° bTDC
Exhaust Valve Opening/Closing	150° aTDC/360° aTDC
Injection System	Bosch Common Rail, P _{max} =1350 bar
Swirl Control/Ratio	AVL/2.0-4.5
Maximum Speed	3000 RPM
Fuel	n-heptane

Table 2. Injector configuration

DI injector Type	Piezo (Continental)
Design	VCO-Nozzle
Angle of Fuel-Jet Axis (inclusive)	142°
Number of Holes	7
Hole Diameter	0.115 mm

Optical Access

Optical access to the combustion chamber is provided through a 20 mm-thick sapphire window mounted in a classic Bowditch extended piston as shown in Figure 3. A mirror inside the piston assembly at 45° relative to the cylinder axis reflects irradiation from the combustion chamber to the measurement device placed on a vibrationally isolated bench top. Both the piston crown and top cylinder liner are mounted with four 14.5×8 mm fused-silica (quartz) windows which allow the introduction of a laser beam into the combustion chamber. Slotted graphite rings provide oil-less lubrication and gapless bronze-teflon rings are used for sealing. Compressed shop air directed at the underside of the piston window cools the assembly during engine operation.

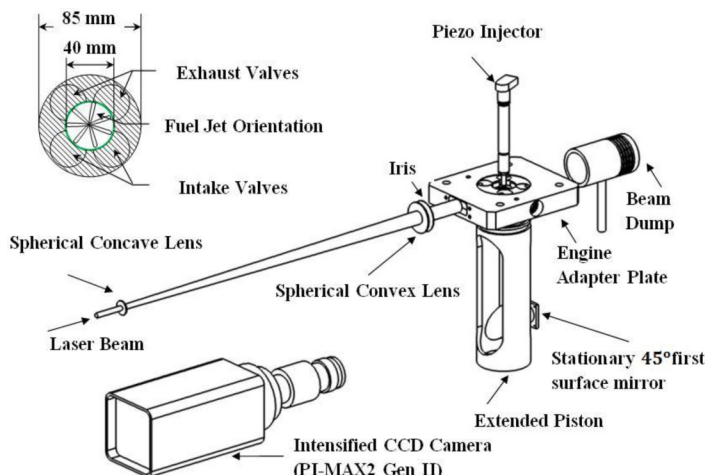


Figure 3. A schematic of engine optical access and Mie-Scattering experimental setup

Liquid Spray Mie Scattering

Figure 3 also shows the Mie scattering layout for liquid spray penetration length measurement. A 532 nm laser beam is generated from the frequency-doubled output of a pulsed Nd:YAG laser (Spectra-Physics Quanta-Ray INDI-40-10). With the second-harmonic generator optimized for the best conversion efficiency, the output is approximately 55.9 mJ per pulse measured at the Nd:YAG laser output. Characterized by a Gaussian profile, the 8 mm diameter laser beam is expanded into a horizontal laser beam of 20 mm diameter using a spherical concave ($f = -400$ mm, Lattice Electro Optics, UF-PC-25.4-400) and spherical convex ($f = 1000$ mm, Lattice Electro Optics, UF-PX-50.8-1000) lens pair. An iris is adjusted to isolate the middle section of the Gaussian beam profile, creating a relatively uniform light beam. Truncation of the laser beam edges with the iris serves to minimize reflections within the side window mount cavities. This laser beam is aligned parallel to the fire deck and is delivered through the combustion chamber via a series of flat fused silica windows mounted both in the adapter plate separating the cylinder head from the crank-case, and the piston crown. This configuration results in laser beam access to the piston bowl around firing TDC, from -27° aTDC to 27° aTDC. The elastic laser signal is acquired by an intensified CCD camera (Princeton Instruments PI-MAX2, GEN II intensifier, 512×512 pixels, 16-bit image depth) once every engine cycle. The ICCD camera is aligned with the axis of the extended piston through a stationary 45° first surface mirror and sapphire window in the bowl. The aperture ratio of the ICCD lens was set to $f/4.0$, and the gain was set to an intermediate value to avoid saturation while maintaining high signal to noise ratio. A field-programmable gate array microprocessor (National Instruments cRIO/DRIVVEN Inc.) is used to trigger a delay generator (Stanford Research DG535). The delay generator then provides triggers for the Q-switch, the laser lamp and ICCD camera gate. The width of the detection gate was kept at 65 μ sec, overlapping the laser elastic signal to overcome the inductive electrical interference present during firing of the piezo injector. In such a configuration, the camera's field of view covers the 40 mm diameter combustion bowl.

Data processing for the Mie Scattering images was conducted with an in-house developed Matlab code. First, a 10 cycle averaged background image with laser pulsing was used to subtract the laser scattering signal from the raw image and then the location of each image pixel with an intensity above the liquid threshold (5% of maximum intensity) was determined for each spray. Liquid lengths were calculated for each plume as the resulting distance from the injector orifice to the spray tip. The penetration lengths are then corrected by the inverse of cosine (19°) to account for the 142° included spray angle and to provide the linear distance from the nozzle tip along the axis of the jet. Finally, average liquid lengths were ensemble averaged from 50 cycles considering only one of the spray plumes in the laser path for all three fuels. The error bars show the standard deviation of the liquid lengths over the 50 cycles.

Broadband Chemiluminescence Imaging

Broadband natural chemiluminescence is acquired prior to high temperature combustion by an ICCD camera (PI-MAX2) once every engine cycle. To maximize the signal to noise ratio, the intensifier gain was set to the maximum value of 250, and the 65 μ sec exposure

time was used with no filtering. A 3-element, ultraviolet lens (Electrophysics) of 78 mm focal length and maximal aperture f/3.8 was used for light gathering. Although the source of emission can be a range of species, including CH*, OH*, C2*, HCO*, PAH or soot incandescence, broadband natural chemiluminescence prior to high temperature combustion has been observed in this and other laboratories to be dominated by CH2O* [27,28,29].

OH Chemiluminescence Imaging

OH* natural chemiluminescence is acquired with the same ICCD camera (PI-MAX2) and setup. An interference band pass filter of 10 nm FWHM having a center wavelength of 307.1 nm was used to isolate OH* chemiluminescence from other emission bands. The aperture ratio of the lens was again set to the maximum opening of f/3.8, and intensifier gain was set to the maximum value of 250. Although generally superimposed on an underlying continuum, the OH* signal is assumed to be the dominant contributor to emission in the 309 nm region.

Due to the limitation of the ICCD camera frame rate, only one chemiluminescence image can be obtained per cycle. For statistical analysis, imaging from the same crank angle was repeated for 30 cycles, and a normally distributed probability density function was used to calculate the maximum probability value of each individual pixel at a given crank angle.

UHC, NO and Soot Emission Measurements

Exhaust UHC was sampled by a fast flame ionization detector (FID) (Cambustion), calibrated against a 5000 ppm propane in nitrogen calibration gas. A fast NOx analyzer (Cambustion) was used to measure NO emission after calibration against 1000 ppm NO in nitrogen. Since the optical engine was skip-fired, a cycle-based exhaust analysis was used. Due to the unsteady mass flow during the exhaust valve opening period, an instantaneous mass flow rate correction method was applied [30]. By assuming the exhaust gas remaining in the engine cylinder undergoes an isentropic expansion during the exhaust valve opening period, the mass trapped in the cylinder changes with crank angle by:

$$m_i = m_{i-1} \left(\frac{p_i}{p_{i-1}} \right)^{\frac{1}{\gamma}} \left(\frac{V_i}{V_{i-1}} \right) \quad (1)$$

Where i-1 and i represent conditions at two successive time steps defined by p, m, r and V, respectively the cylinder pressure, mass, heat capacity ratio and volume. The heat capacity ratio was determined by plotting the P-V diagram and taking the slope of the linear portion of the curve during the expansion stroke. Exhaust mass flow rate then can be calculated using the following equation:

$$\dot{m}_{exh} = \frac{m_i - m_{i-1}}{\text{time per crank angle}} \quad (2)$$

The mass average of a given mass fraction of exhaust gas species k can be determined from the following equation:

$$\bar{x}_{species\ k}^{mass\ average} = \frac{\int_{EVO}^{EVC} x_{species\ k}(t) \dot{m}_{exh}(t) dt}{\int_{EVO}^{EVC} \dot{m}_{exh}(t) dt} \quad (3)$$

Soot measurements were obtained with a smoke meter (AVL model 415s). During data post-processing, the end of each skip-fired pattern was identified by the change in slope of the smoke meter output, from negative to positive, as measured from two consecutive data points. Integration of the data over each skip-fired pattern and the ensemble average were then performed. All three emission analyzers were warmed for approximately one hour prior to measurements to stabilize the thermal condition of the emission equipment. To insure the data was not affected by sensor signal drift during the test, a second zeroing and spanning calibration was performed at the end of each test point.

FUELS

Jet-A (POSF 4658) and its surrogate, mixed from pure compounds, were used for all experiments. N-heptane was also used in the spray measurements as a reference. The surrogate formulation applied here was determined using the surrogate optimizer developed by Kim *et al.* [31]. In the present work, the derived cetane numbers (DCN) of the target fuel and the pure surrogate components were updated within the optimizer with direct measurements from Ignition Quality Tester (IQT) experiments [32, 33]. The DCN's were updated with values obtained from a single source to remove potential device-to-device errors in DCN. After these updates, summarized in Table 3, the relative surrogate composition (n-dodecane/iso-cetane/decalin/toluene) was re-optimized to match the target fuel DCN value, while maintaining similar levels of emulation for the other target properties (MW, LHV, H/C, density, viscosity, surface tension, distillation curve) shown in Figure 4. The resulting surrogate composition was n-dodecane/iso-cetane/decalin/toluene = 0.456/0.145/0.263/0.1358 by liquid volume, with the surrogate DCN within 0.5% of that of the target Jet-A fuel.

Table 3. Measured DCN of the pure surrogate components, target and surrogate fuels (Jet-A POSF-4658).

Fuel	DCN
n-dodecane	76.1
iso-cetane	15
decalin	31.45
toluene	-0.6
Jet-A POSF-4658 (target fuel)	45.02
Surrogate	45.23

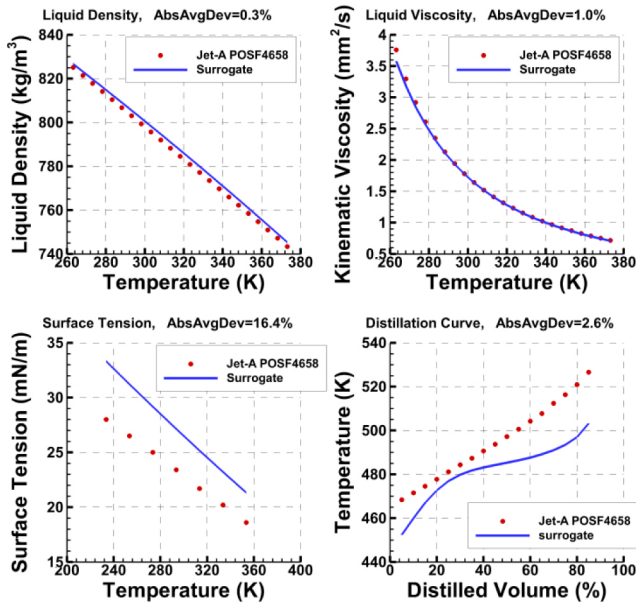


Figure 4. Physical properties of Jet-A POSF 4658 and its surrogate fuels used in the experiments.

ENGINE OPERATING CONDITIONS

During the experiments, the engine oil and coolant temperatures were controlled to 60 °C using an electronic conditioning unit to maintain wall temperature, while the fuel temperature was maintained at 25 °C using process cooling water. The engine speed was kept at 1200 RPM to match the 10 Hz frequency of the laser pulse during the Mie Scattering experiments. The chemiluminescence experiments were conducted with a 20/3 motored/fired ratio to maintain the thermal stability of the engine.

To avoid combustion luminosity inference with the Mie Scattering signal, a non-combusting condition was selected for the spray measurements. This was achieved by retarding the start of injection until autoignition consistently failed. Table 4 shows the same intake and injection conditions for all three fuels.

Table 4. Operating conditions for Mie Scattering experiments

Mie Scattering Experiments	
Injection Pressure	800 Bar
Injector Energize Duration	0.25 msec
Injection Timing	-5° aTDC
Intake Temperature	40 °C
Estimated Isentropic Compression Temperature at SOI	772 K
Charge Density at SOI	19 kg/m ³

To minimize window fouling and signal attenuation, broadband and OH chemiluminescence images were taken at two non-sooting engine conditions, as shown in Table 5.

Table 5. Operating conditions for chemiluminescence imaging

Broadband and OH Chemiluminescence Imaging		
Injection Pressure	800 bar	
Injector Energize Duration	0.35 msec	
Estimated Isentropic Compression Temperature at SOI	837 K	906 K
Charge Density	19 kg/m ³	25 kg/m ³

The degree to which the surrogate represents the behavior of the target fuel over a range of intake conditions was examined with a single injection event for different charge densities at the start of injection (SOI), as shown in Table 6. For each charge density, a range of temperatures and densities at SOI was achieved by controlling the intake air temperature and pressure. CA50 was held constant at about 9° aTDC through the adjustment of injection timing.

Table 6. Operating conditions to assess the effect of intake manifold conditions

Effects of Intake Conditions			
Charge Density at SOI (kg/m ³)	19	25	31
Intake Temperature (°C)	65 to 120	65 to 120	65 to 120
Isentropic Compression Temperature (K)	837 to 981	843 to 980	844 to 976
Injection Timing (°aTDC)	-4 to -0.6	-1.2 to 1.7	0.5 to 3.4

A sweep of injection pressures (400, 600 and 800 bar) was performed at each of the four extreme intake conditions in Table 6 at light load with a single injection. Under these conditions combustion occurred in a primarily premixed manner. A double injection strategy was also used at the same manifold conditions to limit cylinder pressure rise rates. Thus, higher loads could be achieved to examine the fuel behavior in a more diffusion-controlled environment. Similar to the previous chemiluminescence study, CA50s were maintained at 9° aTDC. The current duration of the single and first injections was held approximately constant, while the dwell times for the second injection of the double injection experiments were selected so that the second injection began after the start of combustion. The current duration of the second injection was adjusted to maintain an IMEP of 2.9 bar, while the IMEP for the single injection cases was approximately 1.2 bar. Six cases were examined at each of the four intake conditions, with details for one shown in Table 7. Details for the other cases can be found in the Appendix.