

Effects of Fuel Physical Properties on Auto-Ignition Characteristics in a Heavy Duty Compression Ignition Engine

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ABSTRACT

The effect of fuel physical properties on the ignition and combustion characteristics of diesel fuels was investigated in a heavy-duty 2.52 L single-cylinder engine. Two binary component fuels, one comprised of farnesane (FAR) and 2,2,4,4,6,8,8-heptamethylnonane (HMN), and another comprised of primary reference fuels (PRF) for the octane rating scale (i.e. n-heptane and 2,2,4-trimethylpentane), were blended to match the cetane number (CN) of a 45 CN diesel fuel. The binary mixtures were used neat, and blended at 25, 50, and 75% by volume with the baseline diesel. Ignition delay (ID) for each blend was measured under identical operating conditions. A single injection was used, with injection timing varied from -12.5 to 2.5 CAD. Injection pressures of 50, 100, and 150 MPa were tested. Observed IDs were consistent with previous work done under similar conditions with diesel fuels. The shortest IDs were seen at injection timings of -7.5 CAD. The largest difference in ID between all fuels of $75 \pm 18 \mu\text{s}$ was observed at the earliest injection timing with an injection pressure of 50 MPa. The average difference in ignition delay between individual blends was $35 \pm 18 \mu\text{s}$. None of the blends tested exhibited significant differences in ignition delay compared to the baseline diesel. The results indicate that for the density and temperature range tested, fuel physical properties have limited influence on the ignition process in a heavy-duty diesel engine. Instead, chemical ignition characteristics, i.e., CN, control the ignition delay.

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INTRODUCTION

Forecasted increased demand for diesel fuel and reduced demand for gasoline over the next several decades will drive the need for alternative diesel fuel sources [1]. Suitable alternatives must maintain compatibility with existing infrastructure. The ideal drop-in or fit-for-purpose fuel is one that is inexpensive to produce and requires no modification of engine or refinery hardware for safe, effective operation. Hydroprocessed bio-derived oils and fats and direct sugar-to-hydrocarbon fuels such as farnesane show promise as potential drop-in diesel fuels [2]. Unlike biodiesels composed of fatty acid methyl esters, raw materials such as algae and ligno-cellulosic biomass do not necessarily compete with food production and are relatively abundant. These fuels potentially offer emissions performance that is slightly improved or comparable to existing fuels [3, 4, 5, 6]. Hydroprocessed Renewable Diesel (HRD) fuels based on algal oil have garnered significant attention from the US Navy as a domestically available (and therefore strategically secure) source of marine diesel and jet fuel [7]. Direct sugar-to-hydrocarbon fuels such as farnesane (2,6,10-trimethyldodecane), which is currently in use as a diesel additive throughout Brazil, are also of interest due to their similarity to existing diesel-like petroleum derived fuel components. Farnesane is produced from the fermentation and hydrogenation of the woody portions of sugarcane (a byproduct of sugar production) [6]. These fuels typically have narrow distributions of carbon number or (as is the case with farnesane) are true single-component fuels. Changing from a wide boiling point fuel such as #2 diesel to a narrow

boiling point fuel impacts fuel physical properties such as the distillation curve. Additionally, further changes in physical properties occur if the molecular weight of the alternative fuel is significantly different from that of #2 diesel fuel.

The purpose of this work is to gain a more complete understanding of the critical parameters a replacement fuel must fit to be considered a drop-in replacement in terms of combustion performance. In particular, the relative influence of fuel physical properties as compared to fuel chemistry on ignition and combustion is of interest. The influence of fuel volatility is the primary focus, and the impact of blending narrow boiling fuels of differing volatility with wide boiling petroleum-derived diesel fuel is studied. Narrow boiling ranges are characteristic of many bio-derived diesel fuels. The results of the current work shed light on the impacts of direct use of such fuels and blending with petroleum derived fuels on the ignition and combustion process for conventional diesel combustion.

Background

Ignition Delay

For the purposes of this study, ignition delay (ID) is defined as the interval of time between the start of fuel injection and the start of combustion. ID can be conceptualized as being divided into two distinct parts, a physical delay and a chemical delay. The physical delay is the result of time needed for spray breakup, air entrainment,

and fuel vaporization. It starts at the beginning of liquid fuel injection and ends when sufficient entrainment and mixing has occurred for chemical reactions to become significant. Physical delay is often viewed as being controlled by the physical properties of the fuel, such as: density, specific heat, and volatility [8, 9]. The chemical delay is the result of the autoignition kinetics of the fuel. Chemical delay is heavily dependent on the fuel's molecular structure and associated reactivity. Shock-tube and rapid compression machine measurements with homogeneous pre-vaporized reactants can be used to determine the chemical delay at a set of fixed pressure, temperature, and equivalence ratio conditions [10]. In the engine, the pressure and local temperature and equivalence ratio are time-varying, making it difficult to directly utilize kinetic data to estimate chemical delays in the engine without employing computational fluid dynamics simulations with detailed chemistry.

Both delay processes are dependent on the conditions of the ambient environment at the time that fuel is injected [8]. Reaction kinetics are strongly influenced by temperature. At elevated temperature, faster chemical reaction will occur due to the increased molecular collision frequency and higher energy of collisions. As a result the chemical delay will be decreased [11]. Ambient temperature also affects the physical delay due to the increased rate of thermal energy entrainment. Assuming fixed density, an equal mass of air at a higher temperature transports proportionally more thermal energy when entrained into the fuel jet, resulting in faster evaporation and reducing the amount of entrainment required for significant chemical reaction to occur.

Jet Entrainment Rate

A key factor for both delays is the dependence on the rate of transfer of energy from the surroundings to the fuel. This energy transfer is accomplished by the entrainment and mixing of hot, dense cylinder gasses into the fuel jet. For a quasi-steady diesel fuel jet, the ambient gas entrainment rate is proportional to the ambient density (ρ_a), injector orifice diameter (d_o), injection velocity (U_f), and the tangent of the jet half angle ($\theta/2$) [12], i.e.,

$$\text{entrainment} \propto \rho_a d_o U_f \tan\left(\frac{\theta}{2}\right) \quad (1)$$

Ambient density in an operating engine is dependent on the compression ratio (CR), temperature and density of the intake air, and start-of-injection (SOI) time. Injector discharge characteristics are a result of the geometry of the fuel injector tip. Injection velocity can be estimated using the injector velocity coefficient applied to the Bernoulli equation as shown in Equation (2)

$$U_f = C_v \sqrt{2 \left(\frac{\Delta P_{inj}}{\rho_f} \right)} \quad (2)$$

where C_v is the velocity coefficient of the injector orifice (considered constant for a given injector tip), ΔP_{inj} is the pressure drop across the injector tip (assumed to be the difference between fuel rail pressure and cylinder pressure at the moment of injection), and ρ_f is the density of the fuel. The jet spreading angle θ has been shown to be

dependent on the ratio of the injected fuel's density to that of the ambient gas for quasi-steady fuel jets. Naber and Siebers found the following scaling [12]

$$\tan\left(\frac{\theta}{2}\right) \propto \left(\frac{\rho_a}{\rho_f}\right)^{.19} \quad (3)$$

based on Schlieren imaging measurements performed in a pre-burn type constant-volume combustion chamber. It follows from Equation (3) that an increase in the ambient-to-fuel density ratio caused by either an increase in ambient gas density or a decrease in the fuel density will result in an increased jet spreading angle. Comparison of Equations (2) and (3) indicates that the stronger dependence on fuel density is due to its influence on jet velocity.

Fuel Volatility Impacts on Ignition

The effects of fuel volatility are not included in above relationships. Wong and Steere [13] showed little to no correlation between front end volatility (i.e. the volatility of the first 20% by volume of a fuel) and ignition quality even under cold start conditions. However, their investigation did not involve fuels of the same CN and the resolution of the ignition delay data was relatively poor (80 μ s). They concluded that evaporation of the fuel proceeds in a batch-type distillation manner; with the most volatile components of a fuel evaporating first while the heavier components persist well into the combustion chamber. However, their stated lack of correlation of front end volatility and ignition properties seems to contradict this hypothesis. In the limit of mixing limited vaporization, where droplet breakup and vaporization processes are assumed to be rapid, little impact of volatility would be anticipated on ignition process assuming that heat capacities and enthalpies of vaporization were similar.

Additional investigations of regarding the impact of fuel volatility have been conducted using surrogate fuels. Zheng, et al. [14] studied the effect of volatility on ignition quality for diesel-like fuels in a constant volume combustion chamber and in a rapid compression machine. It was determined that for fuels of matched CN, volatility did not significantly impact the ID, but that fuels of increased volatility did show increased premixed burn intensity. This study focused on jet fuel replacements however, and the span of volatilities was not as broad as in the current work. These findings were later verified in an operating engine [15]. Dumitrescu, et al. [16] also looked at the influence of fuel volatility in their optical engine study that utilized 4 of the Coordinating Research Council Fuels for Advanced Combustion Engines (FACE) diesel fuels. Their work showed little influence of T90 distillation temperature on ignition and they concluded that CN had the largest influence on the engine out emissions and efficiency.

Cetane Number and Chemical Reactivity

The relationship between chemical reactivity and cetane number is complicated, due to the circumstances of both standard test procedures (ASTM D-613 and ASTM D-7668 for CN and DCN respectively) involving both physical and chemical ignition delay processes. In addition, data on isolated chemical reactivity

characteristics for diesel-like fuels is limited. Traditional measurement techniques for quantifying pre-vaporized homogenous charges are ill suited to low-volatility diesel-like fuels, which are prone to thermal decomposition during high temperature charge preparation [17]. However, studies have been carried out using PRF blends similar to those used in the present study as well as with conventional diesel fuels, quantifying ignition quality in compression ignition engines operating under Homogenous Charge Compression Ignition (HCCI) conditions [18, 19, 20]. Such studies utilize either extremely early direct fuel injection at high-pressure, or port fuel injection (PFI) systems to generate a homogenous fuel-air charge prior to the onset of combustion. Under these conditions CN has been shown to correlate well with combustion phasing, and offers a robust metric for predicting fuel chemical reactivity. Similar measurements have been performed recently in our labs using PRF and diesel secondary reference fuel blends. The results of these tests also suggest that under completely premixed-prevaporized HCCI operating conditions fuels with the same CN have the same combustion phasing and hence the same chemical delay. This offers some measure of validity for CN to be interpreted as being closely correlated with the chemical ignition delay, by in large being decoupled from the physical delay (e.g. mixing and vaporization). Based on the results of the above cited studies, in the current study we make the assumption that CN correlates primarily with the chemical delay portion of the ignition delay, and thus assume that fuels with matched CN have approximately matched chemical delay.

Objective

The current work attempts to isolate the effects of physical delay from chemical delay by holding the chemical delay constant, using a fixed CN, while varying the physical fuel properties. The primary fuel property varied is the fuel volatility, although due to the coupling of fuel volatility with other properties, through the molecular weight of the fuel, properties such as viscosity, density, and surface tension vary as well. A range of fuel volatilities are obtained by varying the fraction of two different binary mixtures (one of high volatility and one of low volatility) blended with a baseline #2 diesel fuel. The primary objective is to determine whether fuel volatility (or other properties simultaneously varied) has any significant influence on ignition and combustion when the chemical delay properties are matched under injection conditions where mixing limited vaporization [9] is assumed to dominate. Consistent ambient thermodynamic conditions at the time of injection are maintained for all fuels, but the air entrainment rate does vary between fuels due to variations in fuel density between the baseline diesel fuel and other fuels tested. The influence of this on the entrainment rate and the influence on ignition and combustion is also analyzed and discussed.

EXPERIMENTAL SETUP

Fuels

A 2007 certification diesel fuel with a cetane number (CN) of 45 (Haltermann) was selected as a representative conventional diesel fuel and was used as a reactivity target for the blends used in this investigation. The properties of this fuel are summarized in Table 1. Two different binary mixtures were then blended to match the CN of

the reference fuel: one blend with low volatility and high molecular weight (MW) (with similar average molecular weight as the reference diesel fuel), and the other with lower molecular weight and high volatility. The low volatility binary blend enables the influence of blending a narrow boiling fuel into a wide boiling fuel of similar average volatility/molecular weight to be studied. The high volatility blend allows the influence of blending a narrow boiling fuel with an end boiling point much lower than the initial boiling point of the baseline fuel to be studied. A binary mixture of 70% by volume 2,6,10-trimethyldodecane (farnesane, FAR) and 30% by volume 2,2,4,4,6,8,8-heptamethylnonane (HMN) was used as the high molecular weight, low volatility, blend. The low molecular weight blend was composed of octane number primary reference fuels (PRFs) consisting of 79% by volume heptane and 21% by volume 2,2,4-trimethylpentane (isooctane), commonly referred to as PRF21. The proportions of heptane and isooctane required to achieve a cetane number of 45 were determined using the cetane number versus research octane number (RON) correlation of Kalghatgi [21], i.e.,

$$CN = 54.6 - 0.42 \text{ RON} \quad (4)$$

These fuels were selected due to their structural similarity (all compounds used are saturated alkanes showing various degrees of branching), reactivity, and availability. It should also be noted that farnesane is itself a promising bio-derived alternative diesel fuel [4, 5, 6, 10]. Lubricity improver was added to the binary mixtures (500 ppm of Infineum 661) in equal proportions to prevent damage to the fuel system.

Table 1. Component Properties for Fuel Blends.

Fuel/Fuel Component	n-Heptane	Isooctane	Farnesane [2, 10]	HMN	#2 Diesel [22]	ASTM Test Method
Molecular Formula	C ₇ H ₁₆	C ₈ H ₁₈	C ₁₅ H ₃₂	C ₁₆ H ₃₄	C ₈ -C ₂₁	N/A
Cetane Number	55 [23]	15 [23]	58	15 [24]	45	D613
Molecular Weight	100.2	114.23	212.41	226.44	205 [25]	N/A
Density [kg/m ³]	680 [26]	692 [8]	770	793 [27]	858	D4052
Viscosity [cSt][28]	0.387 (20°C)	0.503 (20°C)	2.33 (40°C)	3.08 (40°C)	2.7 (40°C)	D445
Boiling Point [°C]	98 [26]	98 [26]	198	240 [26]	189-345	D86
Volume % Saturates	100%	100%	100%	100%	65%	D1319
Volume % Olefins	0%	0%	0%	0%	5%	
Volume % Aromatics	0%	0%	0%	0%	30%	
LHV [MJ/kg]	44.66 [26]	44.33 [8]	43.45	43.9 [29]	42.14	D240
H/C ratio	2.28	2.25	2.13	2.125	1.78	D5291

The binary component mixtures, hereafter designated FAR-HMN for the 70% farnesane/30% HMN mixture, and PRF21 for the 79% heptane/21% isooctane mixture, were run neat and blended with #2 diesel in proportions of 25, 50, and 75% by volume. In total, 9 fuels were tested: pure certification diesel, FAR-HMN, PRF21, and the 6



blends mentioned. Density for each blend varied linearly with blend fraction from 858 kg/m³ for #2 diesel to 706 kg/m³ in the case of PRF21 and to 770 kg/m³ in the case of FAR-HMN.

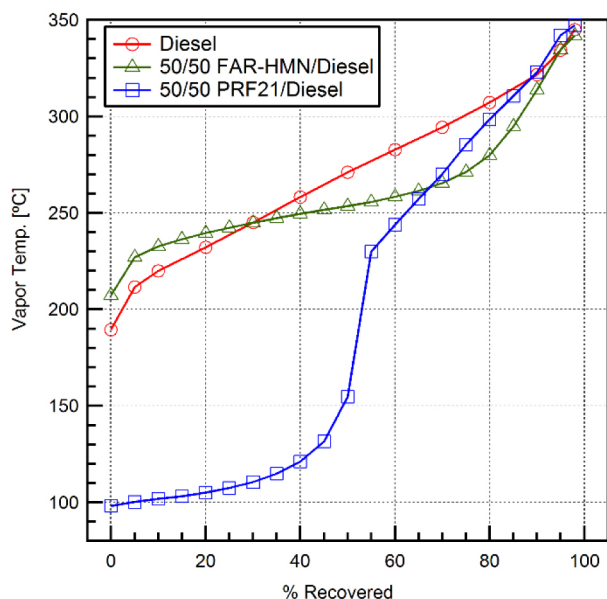


Figure 1. ASTM D86 distillations for #2 diesel reference fuel [22], 50/50 FAR-HMN/diesel blend, and 50/50 PRF21/diesel blend used in this investigation.

Volatility of the blends varied as well, but the change is more difficult to quantify with a single number. As an example, Figure 1 shows distillation data taken in our lab for 2 of the blends and the #2 diesel fuel. The boiling point of both heptane and isooctane is 98-99 °C and a clear distinction is seen in the distillation curve where the high volatility PRF21 is completely boiled away and vapor temperature increases by nearly 100 °C between 45% and 55% volume recovered. The change in temperature at this point roughly corresponds to the difference in initial boiling point (IBP) for PRF21 and #2 diesel. From this we can conclude that blending PRF21 and diesel does not lead to significant molecular interactions affecting the normal boiling points of the pure components.

Similarly with FAR-HMN, the IBP for the mixture is consistent with the lowest boiling point among the individual components. For this blend however, IBP was sensitive to the heating rate and appears to be dominated by farnesane as opposed to the lighter fractions of the diesel fuel. For the 50/50 FAR-HMN/diesel blend the distillation curve is flattened rather than shifted as was the case for the PRF21 blend, since diesel normally contains compounds in the boiling range of FAR-HMN. The flattening of the curve occurs where expected (between 200 and 250 °C) given the boiling points of the blend stock. The flattening is not as complete as it is in the case of PRF 21 due to the presence of compounds of intermediate volatility already present in the diesel. All fuel blends recover the end point (EP) of the pure diesel distillation, indicating the heavier components are unaffected by blending and are simply reduced in concentration by the addition of the binary component mixtures.

From the distillation data we can conclude: 1) fractionally blending diesel with the pure components provides predictable changes in volatility, 2) The volatility of PRF21 and FAR-HMN is consistent with the volatility of the pure species used in blending them, 3) the overall volatility of FAR-HMN is within the diesel boiling point range, and the volatility of PRF21 is significantly higher than that of conventional #2 diesel fuel, which would be required by ASTM D975 to have a minimum vapor temperature of 282 °C at 90% distillate recovered [30]. It should be noted that the blends tested are not intended to meet the specifications of ASTM D975. Specifically, the blends using PRF21 would not meet many of the specifications in the standard, such as those controlling flash point, lubricity, and viscosity. Instead, the current tests are intended to explore the impacts of large changes in fuel properties on conventional diesel combustion and what implications those results may have on the design of future fit-for-purpose fuels.

The blends shown in Figure 1 were also sent out for testing as representative samples for each of the binary component mixtures. Cetane number and density measurements were made following ASTM D613 and D4052 [24, 31]. A third sample of the PRF21 blend was prepared without the lubricity additive and subjected to the same testing to ensure it had no influence on either blend density or CN. All results were consistent with expected values, and the lubricity additive had no impact on fuel reactivity as measured by ASTM D613. Additionally, the assumption of linear blending for CN and density were validated by physical testing. Calculated densities agreed to within 1% and CN values were within 2% of the target (CN 45), which is well within the reproducibility limits stipulated in ASTM D613 [24].

Engine and Laboratory Setup

The engine used in this investigation was a 2.52 L heavy-duty Caterpillar C-15 single-cylinder oil-test engine (SCOTE). Stock cam profiles, valve timing, and piston head geometry were used throughout the testing and are summarized in Table 2. The stock fuel injector was replaced with a Bosch CRIN 2.2 injector body fitted with a 140 µm, 7-hole tip. When using a small injector, the C-15 offers a suitably large cylinder bore to effectively mitigate any piston wetting or spray-wall impingement associated with an injection event, simplifying interpretation of the results.

Pressure data were collected at 0.1 CAD resolution using a piezoelectric in-cylinder pressure transducer (Kistler 6125C20) in conjunction with a charge amplifier (Kistler model 5010B1). Fuel was supplied by a common-rail pump (Bosch CP3) and fuel flow was monitored with a Coriolis flowmeter (Endress and Hauser Promass A83). Air flow to the engine was measured using a 2nd Coriolis flowmeter (Micro Motion CMF 200). Gas species emission data were sampled directly from the exhaust surge tank and measured using a FTIR spectrometer (ThermoScientific Antairis IGS). Sampling was done wet on a continuous basis and passed through a particulate filter to prevent deposits on the spectrometer windows. Molecular oxygen (O₂) was measured after the sample had been dried using a Horiba MPA 210 magneto-pneumatic oxygen analyzer. Soot measurements were taken at a different location, after the exhaust surge tank and pressure control valves and were sampled at the building exhaust

pressure. Intake air was also sampled using the emissions monitoring equipment for each condition. Intake air was provided from building dry compressed air and manifold absolute pressure (MAP) was regulated using a regulator (Proportion Air QB2). Exhaust backpressure was maintained with an adjustable valve. Intake and exhaust gas temperatures were monitored at several locations throughout the air system using type-k thermocouples. Throughout all testing, oil and coolant temperatures were maintained at 90 and 80 $\pm$ 1 $^{\circ}$ C, respectively.

Table 2. Engine specifications and running conditions

Configuration	-Single cylinder -4 valve -Direct injected
Bore x Stroke [mm]	137.0 x 171.0
Compression Ratio	16.3:1
Displacement [L]	2.52
Valve Timing [CAD]	IVC: -154 EVO: 113 IVO: 330 EVC:331
Fuel Injector	Bosch CRI 2.2
Nozzle Hole Diameter [μ m]	140
Included Spray Angle [$^{\circ}$]	148
Number of holes	7
Running Conditions:	
Injection Timing [CAD] (SOI)	-12.5 to 2.5
Injection Pressure [MPa]	50, 100, 150
Speed [RPM]	1300
Load [Bar-IMEP(gross)]	~6
Intake MAP [kPa]	175
Intake Temp [$^{\circ}$ C]	32
Exhaust Backpressure [kPa (absolute)]	190
EGR %	0

The engine was operated at 1300 RPM with an intake pressure of 175 kPa and a temperature of 32 $^{\circ}$ C. Exhaust backpressure was maintained at 190 kPa absolute. Injection timing was swept by changing start of command (SOCmd). SOCmd was defined as the first crank angle, to the nearest tenth, when the injector current trace is greater than or equal to 10% of the maximum injector current draw. Start of physical injection (SOI) was determined by flow rate testing and verified by optical measurements for the same injector body and tip. All injection timings are reported as SOI, corresponding to the start of liquid fuel injection in-cylinder.

Injection durations were varied for each fuel and each injection pressure in order to maintain similar fuel energy injected for each condition. Fuel temperatures were maintained at 17 $^{\circ}$ C at the inlet of the common rail (CR) pump. Fuel was supplied to the CR pump from a 3 gallon stainless steel tank, pressurized to 163 kPa with N₂. Return fuel from the injector and the fuel rail were cooled in a brazed plate heat exchanger and recycled. The heat exchanger and all return lines were also held at 163 kPa. Prior to data collection, the engine was fired for a minimum of one hour on conventional diesel fuel for warmup,

supplied by a larger tank and delivered to the engine via the same CR pump and injector. The fuel system was designed to minimize wetted volume, and to eliminate dead volume where fuel could conceivably collect to reduce operation time needed to expel the remaining #2 diesel in the fuel system when the fuel supply was switched over to the test fuel of interest. Comparisons of heat release and fuel flow-rate data were used to characterize the time necessary to fully clear the system, and no data were collected for 10 minutes following fuel supply switching to ensure complete flushing of the system.

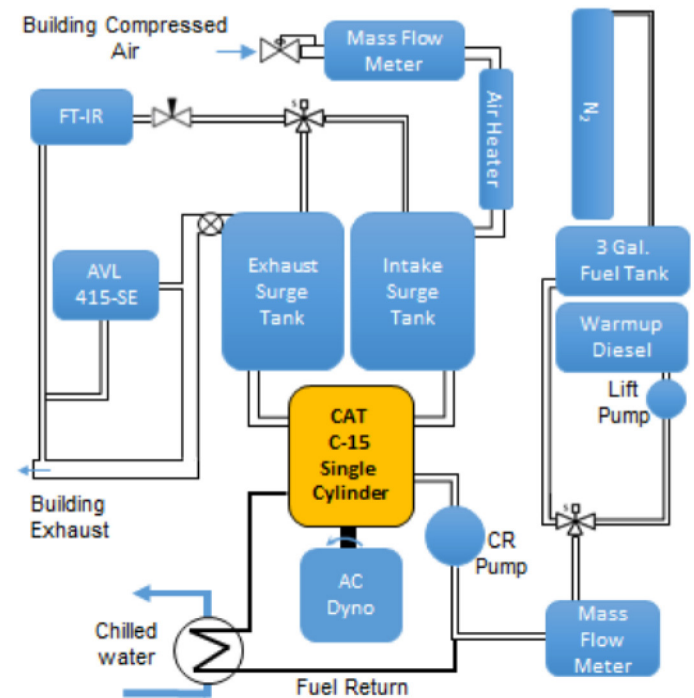


Figure 2. Schematic diagram of engine setup showing air and fuel systems used in this investigation.

Ignition Delay Determination

Ignition-delay measurements in operating engines can be somewhat subjective, and tend to vary based on the ignition delay criterion and data processing used. Before a discussion of the ID data presented in this paper, it is important to understand the calculation technique employed in its determination. Ignition delay in a CI engine is defined as the elapsed time between start of injection and start of combustion (SOC). Start of injection corresponds to the time when fuel begins to enter the engine cylinder which is slightly delayed from the start of injection command, i.e., when the signal is sent to the injector to begin injecting. SOC is more difficult to determine and is based on pressure data collected in cylinder. A number of techniques for determining SOC and their respective merits and drawbacks have been previously described by Rothamer and Murphy [32]. One common approach has been to locate the maximum of the second or third derivative of cylinder pressure with respect to crank angle. A similar method is to determine from heat release analysis when a threshold quantity of fuel energy has been released as sensible energy. These methods are heavily reliant on the quality of the pressure trace, as even small amounts of noise can cause large disturbances in the necessary derivatives. Furthermore, conventional noise reduction