

**TWO-STAGE IGNITION AS AN INDICATOR OF LOW TEMPERATURE
COMBUSTION IN A LATE INJECTION PRE-MIXED COMPRESSION
IGNITION CONTROL STRATEGY**

A Thesis

by

JOSHUA ANDREW BITTLE

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

December 2010

Major Subject: Mechanical Engineering

Two-stage Ignition as an Indicator of Low Temperature Combustion in a Late Injection

Pre-mixed Compression Ignition Control Strategy

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Approved by:

Chair of Committee,	Timothy Jacobs
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ABSTRACT

Two-stage Ignition as an Indicator of Low Temperature Combustion in a Late Injection
Pre-mixed Compression Ignition Control Strategy. (December 2010)

Joshua Andrew Bittle, B.S., Oklahoma State University

Chair of Advisory Committee: Dr. Timothy Jacobs

Internal combustion engines have dealt with increasingly restricted emissions requirements. After-treatment devices are successful in bringing emissions into compliance, but in-cylinder combustion control can reduce their burden by reducing engine out emissions. For example, oxides of nitrogen (NO_x) are diesel combustion exhaust species that are notoriously difficult to remove by after-treatment. In-cylinder conditions can be controlled for low levels of NO_x , but this produces high levels of soot potentially leading to increased particulate matter (PM). The simultaneous reduction of NO_x and PM can be realized through a combustion process known as low temperature combustion (LTC).

In this study, the typical definition of LTC as the defeat of the inverse relationship between soot and NO_x is not applicable as a return to the soot- NO_x tradeoff is observed with increasing exhaust gas recirculation (EGR). It is postulated that this effect is the result of an increase in the hot ignition equivalence ratio, moving the combustion event into a slightly higher soot formation region. This is important because

a simple emissions based definition of LTC is no longer helpful. In this study, the manifestation of LTC in the calculated heat release profile is investigated.

The conditions classified as LTC undergo a two-stage ignition process. Two-stage ignition is characterized by an initial cool-flame reaction followed by typical hot ignition. In traditional combustion conditions, the ignition is fast enough that a cool-flame is not observed. By controlling initial conditions (pressure, temperature, and composition), the creation and duration of the cool-flame event is predictable. Further, the effect that injection timing and the exhaust gas recirculation level have on the controlling factors of the cool-flame reaction is well correlated to the duration of the cool-flame event. These two results allow the postulation that the presence of a sufficiently long cool-flame reaction indicates a combustion event that can be classified as low temperature combustion. A potential method for identifying low temperature combustion events using only the rate of heat release profile is theorized.

This study employed high levels of EGR and late injection timing to realize the LTC mode of ordinary petroleum diesel fuel. Under these conditions, and based on a 90% reduction in nitric oxide and no increase in smoke output relative to the chosen baseline condition, a two part criteria is developed that identifies the LTC classified conditions. The criteria are as follow: the combustion event of conventional petroleum diesel fuel must show a two-stage ignition process; the first stage (cool-flame reaction) must consume at least 2% of the normalized fuel energy before the hot ignition commences.

DEDICATION

To Tiffanie and ALL the rest of my family

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Thank you to all the teachers, advisors, and friends I have had along the way. This is an important step to take, and I am proud to have made it with your help.

Special thanks to my parents, my wife, great lab mates, great advisor, Dr. Jacobs, and committee members, Dr. Caton and Dr. Karpetis.

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1. INTRODUCTION

1.1. Motivation

Since the late 1960's engine exhaust emissions concentrations have been progressively restricted. The development of combustion control equipment and after-treatment devices have successfully meet the legislated requirements. However, further advances in combustion control strategies can help reduce the burden of the after-treatment devices. In relation to diesel combustion, the oxides of nitrogen (NO_x) are well known for their difficulty in after-treatment effectiveness. Combustion conditions in-cylinder can be controlled to limit NO_x formation with ease; however, the act of reducing NO_x increases the soot formation which could produce increased particulate matter (PM).

Other emission species are certainly worthy of concern, but in this study the reduction of soot and NO_x is the focus. Both of these species can have very negative effects on humans and the environment. NO_x is primarily composed of nitric oxide (NO) and nitrogen dioxide (NO_2). Both of which readily react with molecular oxygen (O_2) in the atmosphere. The reaction breaks the O_2 molecule such that one oxygen atom is bonded with the NO_x species and the other is left unbounded. This atomic oxygen left unbounded quickly combines with another O_2 molecule to form ozone (O_3). While ozone in the upper atmosphere is beneficial because of its ability to reflect solar radiation, ozone in the lower atmosphere is harmful to humans. It can cause significant temporary

This thesis follows the style of Journal of Engineering for Gas Turbines and Power.

lung function degradation in the young and old as well as anyone with asthmatic symptoms [1].

The presence of PM in the air can have similar effects to ozone on the human respiratory system. Particulate matter also contributes to decreased visibility through haze formation and environment degradation. The PM suspended in the air can attach to water droplets in the air and form large conglomerates that block visible light – effectively limiting visibility [2]. By atmospheric air currents the PM can be taken from dense urban areas and deposited in the surrounding vegetation areas. In those areas the PM can pollute the water sources, and remove nutrients from the soil [2].

Clearly both NO_x and PM are not a benefit to humanity or the environment. Under conventional combustion only one of these can be reduced effectively in the engine. The use of diesel particulate filters and NO_x traps have been successful at meeting emissions regulations. However future emissions standards are only making these after-treatment systems more complicated and expensive.

The simultaneous reduction of NO_x and PM can be realized through a combustion process known as low temperature combustion (LTC). While operating in a LTC mode does have drawbacks, the most important advantage, the successful simultaneous reduction of NO_x and soot, has great potential for simplifying the after-treatment systems needed for diesel operation [3-4]. This type of combustion has been under investigation since Onishi et al. first discussed the “active thermo-atmosphere combustion” event they studied [5]. While the term used to describe this type of combustion has changed many times, the ultimate goal is to eliminate NO_x and soot

formation. The simultaneous and substantial reduction of NO_x and soot has been demonstrated many times [6]. The method of LTC attainment will be described shortly – at this point is important to discuss why LTC has not been implemented in production engines.

Despite the benefits of LTC and its repeated demonstration, it is equally common to find the observation that carbon monoxide (CO) and unburned hydrocarbons (HC) both increase substantially as NO_x is reduced [7]. In addition to increased CO, the operational load limitations are well documented, for example [8]. Despite these drawbacks the community research effort targeted at LTC is strong and will likely continue to be so.

Finally, the control strategies utilized to operate in a LTC mode are fairly well documented [6], but applying these to a commercial engine is not simple. While static control maps could be developed, a real-time diagnostic method that provides feedback to the controller would be optimal. Furthering the foundation of knowledge for a potential control strategy of this type provides the motivation for this study. Specifically, a diagnostic parameter that could be calculated only from the in-cylinder pressure measurement of a given engine cycle has been investigated.

The parameter targeted as a LTC diagnostic is the cool-flame reaction duration calculated from the in-cylinder pressure profile. The concept of cool-flame reactions, how LTC is actually realized, and the link between the two are presented next. The objective study will conclude the introduction. This will be followed by the experimental methodology, results and conclusions.

1.2. Background

1.2.1. Cool-flame Reactions

Cool-flame reactions have been thoroughly researched since the initial discovery of the bluish flames appearing over a flask of evaporating ether [9], to the first investigations of the role cool-flames play in engine knock [10]. The peculiar behavior of the cool-flame reactions is well documented. It has been shown that up to five cool-flames could be observed in succession [11]. This is a result of the unusual presence of temperature islands for which the cool-flame reactions possess a negative reaction rate coefficient [12]. That effect is a complicated result; thus some description of a few general reactions and their properties follows to clarify why the cool-flame reaction is significant and then how it is manifested in an engine environment.

In any reversible chemical reaction at a given set of conditions there is a “direction” that the reaction is going to move. This is contrary to an irreversible reaction that can only proceed in one direction. Regardless of the type of reaction, its speed can be characterized by a reaction rate. An irreversible reaction can only occur in one direction and thus can only have a positive reaction rate. Contrarily, a reversible reaction can occur in both a forward and backward manner. This gives rise to a positive and negative reaction rate corresponding to a forward and backward reaction direction respectively.

While the reactions involved in cool-flame reactions and combustion in general are quite complex, they can be simplified for discussion if all long chain fuel molecules

are simply represented by “RH”. The first three reactions that can occur will be shown and discussed to help explain how multiple cool-flames can be observed.



The first reaction (1) removes a hydrogen atom from the chain. This reaction has a large activation energy, which means that it requires a large amount of energy in order for the hydrogen atom bond to be broken [13]. If an adequate amount of energy has been delivered and an oxygen molecule collides with the fuel chain the hydrogen atom will break off of the fuel chain and combine with the oxygen molecule. This reaction is irreversible because the bond created between the oxygen molecule and the freed hydrogen atom will only be broken by another significant energy addition. The removal of the hydrogen atom leaves the fuel chain with an open bond site. This open bond site classifies the fuel chain as a radical. A radical in any form is a molecule that will react readily. Therefore at this point the reaction will proceed to either (2) or (3) depending on the conditions.

Reaction (2) is the primary cool-flame mechanism. It has three important characteristics – it has negligible activation energy, is exothermic in the forward direction and is reversible [13]. The first property (negligible activation energy) means that this reaction will proceed if there is a fuel radical available. The second property (exothermic in forward direction) means that when the oxygen molecule combines with

the fuel radical heat is released. The third property (reversible) means that the reaction can occur both forwards and backwards.

Reaction (3) is the fuel chain breaking reaction that leads to the eventual hot ignition, that which is typically thought of when discussing combustion. The long fuel chains are broken down into simpler hydrocarbons that ultimately “burn”. This process has large activation energy and thus only occurs at a significant rate at higher relative temperatures to that of reaction (2) such that in that typically either one or the other occurs at any given time [13].

Reaction (2) is of primary importance in this study as it helps describe some of the properties of the cool-flame reactions. As the reaction first proceeds the exothermic nature will cause the temperature of the mixture to increase. However, due to the temperature islands for which reaction (2) has a negative reaction rate, if conditions are favorable the reaction will reverse and the temperature will start to decrease. The mixture temperature will change the reaction direction to a forward direction again. This once again will increase the mixture temperature. As the reaction proceeds, the shift from positive to negative reaction rates result in the multiple cool-flames. The chemistry is more complicated than shown here, but the general idea has been conveyed.

The multiple cool-flame reactions are not observed in engine reactions. The experimental setups that are able to demonstrate multiple cool-flames are constant volume homogeneous mixture reactors. In those experiments the only thing changing the reaction pressure or temperature is the chemistry. In an engine environment the piston motion is either increasing (compression) or decreasing (expansion) the temperature.

While the cool-flame reactions do consume some amount of fuel, the effect of the piston motion does not allow for the reaction rate reversal that the constant volume reactor provides. Under specific conditions such as those in an engine, however, the cool-flame reaction could elevate the mixture to a state where a hot ignition event takes place [14]. Two-stage ignition occurs when, under typical conditions, only a single cool-flame reaction is observed and is followed by hot ignition [15]. This phenomenon is what occurs in the knocking behavior of engines, and is also the type of cool-flame reaction under study here.

Spark ignitions engines by definition control ignition through the use of a spark. If conditions are such that the fuel mixture reaches temperatures where ignition will occur without the presence of a spark then auto-ignition will occur. This is undesirable because it causes both large pressure increases, which can damage the engine, and uncontrolled combustion phasing, which can negatively affect efficiency and power. The auto-ignition event in spark ignition engines can be delayed and potentially eliminated by the presence of a cool-flame reaction. While some fuel is consumed in the cool-flame reaction it is not enough to cause significant temperature and pressure changes in the engine cylinder. If the duration of the cool-flame reaction could be increased the auto-ignition could be delayed long enough for the spark ignited combustion to occur first. In compression ignition engines the auto-ignition properties of the fuel are used to control combustion. This is contrary to spark ignition engines in which auto-ignition is undesirable and is termed “knock” as described above. The behavior of the cool-flame reaction is still interesting to consider in a compression ignition event due to the

possibility that a significantly long cool-flame reaction could be used as an artificial ignition delay mechanism when a two-stage ignition occurs.

1.2.2. Low Temperature Combustion Attainment

Both soot and NO_x are heavily dependent on combustion temperature and equivalence ratio. The simplified description of the method used in most LTC control strategies is the addition of EGR as both a diluent and an ignition delay modifier. As a diluent the more EGR present in the mixture the lower the combustion temperatures. The EGR (a diluent) acts as a heat sink for the combustion reaction. Since the EGR is non-reactive it simply absorbs the reaction heat such that reaction temperatures are limited. The secondary effect of increased ignition delay does not directly affect the combustion temperature (it does so indirectly by changing combustion phasing), but it does change the ignition equivalence ratio. A longer ignition delay means more mixing time and thus a lower equivalence ratio. Keep in mind that while diesel combustion and especially LTC are characterized by a lean mixture, the direct injection system creates a non-homogeneous mixture. This means that despite the overall lean mixture, the regions of combustion will be locally rich. This is important to remember when looking at Figure 1 to understand how lower temperature and equivalence ratio can result in lower emissions formation.

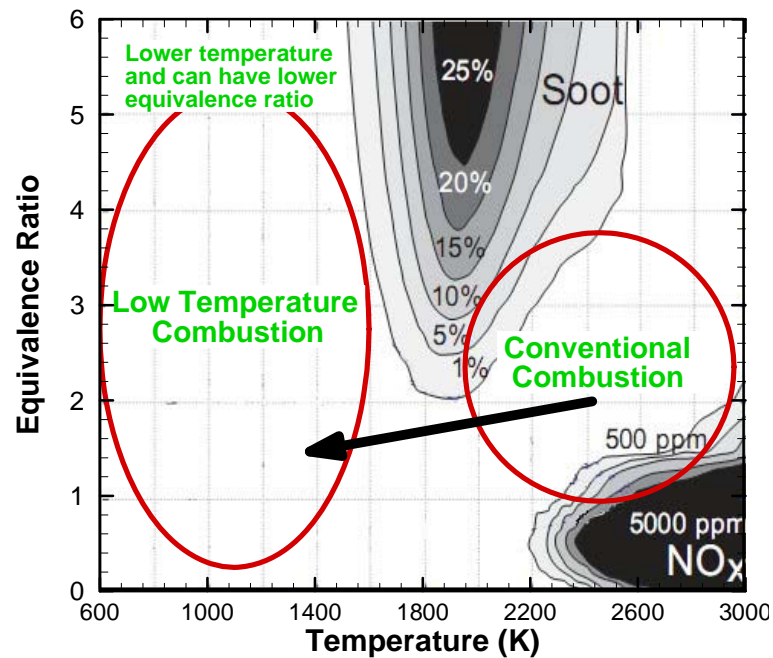


Figure 1 Emission formation as a function of temperature and equivalence ratio. Adapted from [16] based on work done by [17].

Notice in Figure 1 how the soot and NO_x are both functions of temperature and equivalence ratio. As described, the addition of EGR decreases the combustion temperatures and can, though it does not always, decrease the equivalence ratio when LTC is realized. It is clear how these two changes both decrease the soot and NO_x formation.

1.2.3. Link between Cool-flame and Low Temperature Combustion

Like the investigations in to cool-flames and knock behavior, this study investigates the cool-flame reactions behavior in a compression ignition engine operating in a LTC mode.

The foundation for the study presented here is the work published in 1969 by Fish et al., which is an experimental study of the cool-flame reaction and the parameters that influence its behavior [14]. The test apparatus of that study is a rapid compression machine inducting a homogeneous charge of fuel and air. [14] report a strong correlation between cool-flame duration behavior, initial pressure and equivalence ratio. It is interesting to remark that one of the conclusions reached by Fish et al. reads: "Reduction of the intensity of the cool-flame reaction may well be the key to effective anti-knock action"[14]. The cause of the knock is high ambient temperature auto-igniting the mixture. Eliminating knock is traditionally achieved by combining constrained compression ratio with an increased octane fuel. A reduced compression ratio reduces the in-cylinder pressures and thus temperatures; the increased octane rating of the fuel increases the resistance to auto-ignition. The discussion by Fish et al. combines these two effects. By controlling the cool-flame duration (through manipulation of temperatures and pressures) the auto-ignition resistance could be artificially increased such that the unburned mixture does not reach temperatures required for hot ignition as quickly. Ultimately the goal would be to reduce the temperature to avoid knock - this result is precisely the goal of low temperature combustion.

That discussion is focused on spark ignition applications. In direct injection compression ignition engines the ignition timing is controlled by utilizing the ignition delay combined with injection timing. Traditionally the implementation of LTC is realized by increasing EGR, and also ignition delay to the point where combustion temperatures are decreased as described in the previous section. By using conditions that

favor cool-flame reactions the ignition delay can be effectively increased beyond the effect of EGR addition. The link between cool-flame reactions and ignition delay suggests that if the cool-flame duration was substantial enough to delay combustion then LTC attainment could be observed.

1.3. Objective

Generally in research conditions emissions analysis equipment is used to verify or determine if the engine is operating in a LTC mode. This equipment is currently too large and expensive to consider including on board a vehicle at this time. Alternatively it is possible to include the relatively simple equipment needed for in-cylinder pressure measurement; for example, Audi has implemented a combustion sensor that provides feedback control in its 2008 high-pressure common-rail 3.0-L TDI engine [18].

As such, the objective for the study is to determine if an in-cylinder pressure measurement could be used to diagnose an operating condition as either LTC or not. Ideally a general method would be used, but an engine or condition specific method may be required. As a first step in this work, a late injection high exhaust gas recirculation (EGR) strategy is investigated.

2. EXPERIMENTAL SETUP AND METHODOLOGY

2.1. Engine and Dynamometer

The engine used in this study is a four cylinder medium-duty diesel engine. Of particular importance are a few advanced technologies which enable the pursuit of this study's objective. These technologies include a high pressure common rail fuel system supplying electronically controlled direct injection fuel injectors, a variable geometry turbocharger, and a cooled EGR system. Relevant engine specifications are listed in Table 1. The fuel used in the test is a standard Diesel #2, with certain properties (and associated test standard) given in Table 2.

In order to realize the LTC mode, this study makes use of a custom full authority engine controller produced by Drivven, Inc. of San Antonio, Texas, USA. This system allows for individual, independent control of all the engine electronic sub-systems. This means that the injecting timing and EGR valve position – i.e., the controlled parameters of the study – can be set and maintained.

The test engine is coupled to a DC motoring dynamometer (dyno). The dyno loads the engine via automatic feedback control adjustment of the field current to maintain the desired engine speed.

Table 1 Specifications of the medium-duty engine apparatus under investigation.

Bore	106 mm
Stroke	127 mm
Displacement	4.5 L
Rated Power	115 kW at 2400 rev/min
Compression Ratio	16.57 ^a (nominally 17:1)
Ignition	Compression
Fuel System	Electronic common rail, direct injection
Air System	Variable geometry turbocharger with EGR

^a Measured by oil displacement

Table 2 Summary of the properties of the fuel used in this study.

Property [Standard]	Diesel #2^a
Density (kg/m ³) [ASTM D4052s]	825.5
Net heat value (MJ/kg) [ASTM D240N]	43.008
Gross heat value(MJ/kg) [ASTM D240G]	45.853
Sulfur (ppm) [ASTM D5453]	5.3
Viscosity (cSt) [ASTM D445 40C]	2.247
Cetane Number [ASTM D613]	51.3
Hydrogen (%-mass) [SAE J1829]	13.41
Carbon (%-mass) [SAE J1829]	85.81
Oxygen (%-mass) [SAE J1829]	0.78
Initial boiling point (°C) [ASTM D1160]	173.4
Final boiling point (°C) [ASTM D1160]	340.5

^a Measured or Calculated by Southwest Research Institute (San Antonio, Texas)

2.2. Experimental Test Matrix

Two injection timings are evaluated: a timing of -8° aTDC (after top dead center), which is termed the “conventional” timing and a late timing of 0° aTDC which is termed the “late” timing. The fuel injection duration is set at the conventional injection timing with zero EGR to achieve a torque load of 68 N-m while the dyno controller maintained a speed of 1400 rotations per minute (RPM). The fuel injection duration is held constant for each test condition with a constant controlled rail pressure of 816 bar (this rail pressure is the factory calibrated setting for this speed and load).

A sweep of the EGR valve position is performed for both injection timings while holding all other control settings constant. As a result of the production engine used in this study, holding the control settings constant does not allow for the constraint of parameters such as EGR temperature, manifold pressures, and air flow rate. It is important to consider again that this study uses a production engine. If a control strategy such as the one used in this study was to be implemented commercially the changes in EGR temperature, manifold pressures and all other parameters would be uncontrollable side effects. Consumer engines do not have systems that keep these parameters constant, so while these changes could create differences between this studies results and a hypothetical similar study performed on a fully equipped research engine, this behavior change increases the validity of the studies potential application to a consumer engine.

2.3. Measurements and Data Acquisition

Several measurements are used to provide data for analysis in the study. The most important of these is in-cylinder pressure. In-cylinder pressure is measured from

cylinder #1 (the forward most cylinder) on a crank-angle resolved basis (0.2 degree resolution) using a piezo-electric based pressure transducer. The ordinary calibration and fidelity checks were done for this measurement [19]. This measurement is collected for 300 consecutive cycles; analysis is performed on the averages of the 300 cycles to remove cyclic variation and get a good measurement of the true steady-state operation.

Other measurements include brake torque (using a load cell), fuel flow rate (using a positive displacement meter), exhaust nitric oxide concentration (using a chemiluminescence technique), exhaust smoke concentration (using a reflective smokemeter technique), exhaust hydrocarbon concentrations (using a flame ionization detection, and reported on a propane basis), exhaust carbon monoxide concentration (using a non-dispersive infrared technique), and intake and exhaust carbon dioxide concentrations (using non-dispersive infrared techniques, and are used to determine EGR level). Exhaust samples for gaseous and smoke speciation were delivered to the respective analyzers through either sample lines that were heated to 190°C (NO, hydrocarbon, and smoke analyzers) or cooled and dehumidified (carbon monoxide and carbon dioxide analyzers).

Calibration of all instruments is routinely conducted to minimize systematic uncertainty. Random uncertainty in engine testing can be high, because of a number of ambient factors, such as temperature and humidity. Repeated testing of operating conditions and combustion regimes (i.e., multiple sets of measurements) over several days go into each set of data, of which statistical analysis is performed using standard techniques [20]. The uncertainty bars in the data figures are the result of this analysis.

Finally, in some figures such as those showing exhaust species concentration data, lines connecting data points are meant to illustrate the series of data, and do not suggest a trend between data points.

2.4. Calculations

2.4.1. Exhaust Gas Recirculation

This study used two injection timings with sweeps of EGR at each. The control setting used to change the EGR level is the EGR valve position. However, the important parameter for comparisons between injection timing is the actual EGR mass percent. To make this calculation the exhaust species concentration and the intake manifold carbon dioxide (CO₂) concentration must be known. Only the species with relatively high concentration are used to simplify the calculation. These include nitrogen, oxygen, CO₂, water (H₂O) and CO.

This is a fairly standard calculation that is implemented as described in Heywood using the suggested value for the equilibrium constant [21]. The equations used are included and summarized below.

The definition of EGR is the total mass fraction of the exhaust species present in the intake. In the equation below, ‘X’ represents the mass fraction of the individual exhaust species’.

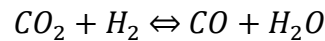
$$EGR\% = \sum_{intake} X_{exhaust,i}$$

Calculating this value requires converting concentrations to molar and then to mass fractions. The conversion between molar and mass fraction for each species is

accomplished with the following equation, where ‘X’ represents mass fraction, ‘Y’ represents molar fraction and ‘MW’ represents molecular weight.

$$X_{exhaust,i} = \frac{Y_{exhaust,i} \cdot MW_{exhaust,i}}{MW_{EGR}}$$

The H₂O levels are calculated using water-gas shift equilibrium reaction mechanism.



This balance reaction allows for the equilibrium molar concentrations of the involved species to be determined as a function of an empirical equilibrium constant. For engine conditions the constant, ‘K’, value is taken as 3.8 based on the recommendations in [22]. In this application the equilibrium equation, shown below, is used to calculate the water concentrations in the intake and exhaust.

$$Y_{H_2O} = \frac{CO + CO_2}{1 + \frac{CO}{K \cdot CO_2} + \frac{M}{2N} \cdot (CO + CO_2)}$$

In the case of the intake water calculation it is assumed that the ambient CO concentration is negligible.

Finally, the ratio of ‘M/2N’ is based on the fuel type used.

Based on the calculated water concentration, the species concentrations are converted from a dry basis (how they are measured) to a wet basis to allow for a true mass fraction calculation. Then besides the calculation of the water concentrations (which is necessary since these values are not measured directly during data acquisition),

the remainder exhaust species intake concentrations are determined based on the CO₂ dilution ratio. This dilution ratio is defined as the ratio of intake CO₂ to exhaust CO₂.

2.4.2. Apparent Heat Release Rate

In-cylinder pressure is used in the calculation of rate of heat release. A digital filter is employed to remove high frequency noise from the raw pressure measurements to provide relatively smooth rate of heat release profiles. Under the assumption of a single zone mixture and ideal gas behavior, the rate of apparent heat release is calculated using the First Law of Thermodynamics. The following summary is an overview of the calculation method.

The energy balance, which tracks all energy transfers and storage in the cylinder, is shown below. This equation is followed by an illustration of the control volume in Figure 2 which defines sign conventions and shows how each term can influence the heat release rate. The balance of these energy terms maintains the energy conservation criteria of the 1st Law of Thermodynamics. The terms in respective order are the apparent heat release rate, piston work rate, internal energy change rate, and heat transfer rate.

$$\delta Q_{HR} = -\delta W + dU_{cv} - \delta Q_{HT} \quad (4)$$

The work term accounts for the work done by or on the piston as the cylinder contents are compressed or expanded, respectively. A positive work term (work during the expansion stroke) decreases the calculated heat release rate. The internal energy term accounts for the change in energy storage of the cylinder contents as the temperature changes. An increase in internal energy (generally the same as an increase in

temperature) of the mixture increases the calculated heat release rate. The heat transfer term tracks the heat energy transfer either from or to the surroundings (such as the cylinder walls). A heat transfer to the surroundings decreases the calculated heat release rate. Finally, due to the combustion event there is an increase in cylinder energy, termed heat release that is modeled simply as another heat transfer source. In reality, the energy release is due to chemistry mechanisms in the cylinder. However, including the detailed chemical kinetic mechanisms would add unnecessary complication to the calculation which is intended to be simple. The simplification of modeling the combustion as a simple heat transfer source is the reason the calculation is termed ‘apparent’ heat release.

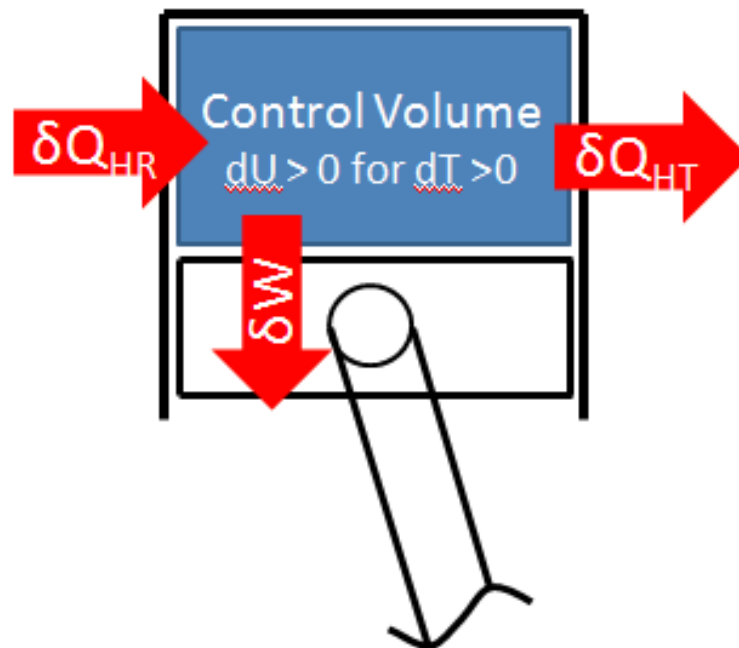


Figure 2 Heat release control volume definition.

Equation 4 is rearranged to solve for the heat release term, dQ_{HR} . This means that the remaining three terms must be calculated in order to get the desired dQ_{HR} output. The work term is calculated from the cylinder geometry and pressure measurement as follows, where p is pressure and dV is the rate of volume change of the cylinder.

$$\delta W = p * dV \quad (5)$$

The internal energy term makes use of the assumption that the mixture behaves as an ideal gas. In that case, the internal energy is only a function of temperature, and the mixture components individual properties are additive.

$$dU_{CV} = \sum_{species,i} x_i m C_{v,i} dT \quad (6)$$

Equation 6 includes terms for species mass fraction, x_i , total trapped mass, m , species specific heat, $C_{v,i}$, and rate of temperature change, dT . Once again, the ideal gas assumption allows for the use of $C_v dT$ term to calculate each species internal energy change and the use of the summation over each species. The species mass fractions, specific heat, and the temperature change all must be determined individually.

The temperature calculation is a simple application of the ideal gas law. The pressure measurement is combined with the cylinder geometry, known trapped mass, and the mixture gas constant at measured increment to solve the ideal gas law equation for the temperature.

Both the species concentrations and the specific heat values are calculated based on information in the JANAF tables [23]. These computerized tables have detailed equation fits for experimentally determined species properties. Also included in the

tables are species equilibrium mechanism constants that aid in determining the equilibrium concentrations for a specific reaction (such as the water-gas shift reaction described in Section 2.4.1). These equations allow for the simultaneous solution of a number of important species equilibrium mechanisms that are included in the calculation. Subsequently, knowing the species concentrations that correspond to a given temperature and pressure along with the species specific heats allow for the calculation of the mixture internal energy.

The last term, heat transfer, is calculated using a simple heat transfer model.

$$\delta Q_{HT} = m A h d(\Delta T) \quad (7)$$

The trapped mass is known, and the cylinder geometry allows for the calculation of the wall area available for heat transfer. The ΔT term is the difference between the cylinder contents temperature and the wall temperature. For this calculation method the wall temperature is assumed and treated as constant. The tests are run at steady-state conditions, so the assumption that the wall temperature is constant is justified. Finally, the heat transfer coefficient is an additional function of temperature. A well established correlation developed by Hohenberg is utilized in this calculation method [24]. Part of that correlation includes the assumption that for diesel combustion the radiation heat transfer is negligible, thus only the convective heat transfer component shown in Equation HR4 is included.

The validity of these calculation methods have been demonstrated by [25-26]. Additionally, more information on the supporting property calculations can be found in [27-28]. Finally, an important parameter that is part of the heat release rate calculation is

the mass fraction burned (MFB) profile. The heat release rate quantifies the fuel energy released at each increment during the calculation. If this parameter is integrated then the cumulative heat release is obtained as the total fuel energy released at any given point during the combustion process. If this parameter is then normalized by the total fuel energy delivered then the resulting value is the MFB. In other words the MFB profile shows the percent of total fuel energy that has been consumed at any given time.

2.4.3. Cool-flame Property Support Calculations

The most important property to quantify when analyzing the cool-flame reaction is the duration. In the analysis presented here the duration is defined as the crank angle degrees spanned between start of combustion (SOC) and the start of significant heat release. SOC is defined as the location of local minimum heat release point after injection before significant heat release. This point is chosen because it is the point where the energy release becomes larger than the energy absorbed by the fuel during vaporization. The start of significant heat release is taken as the inflection point in the heat release profile that occurs after SOC and before the peak heat release location. The inflection point must occur in a positive heat release position. This stipulation maintains the condition that a cool-flame still represents a positive contribution to the cumulative heat release despite the low intensity of the reaction. Figure 3 shows an illustrative explanation of this calculation.

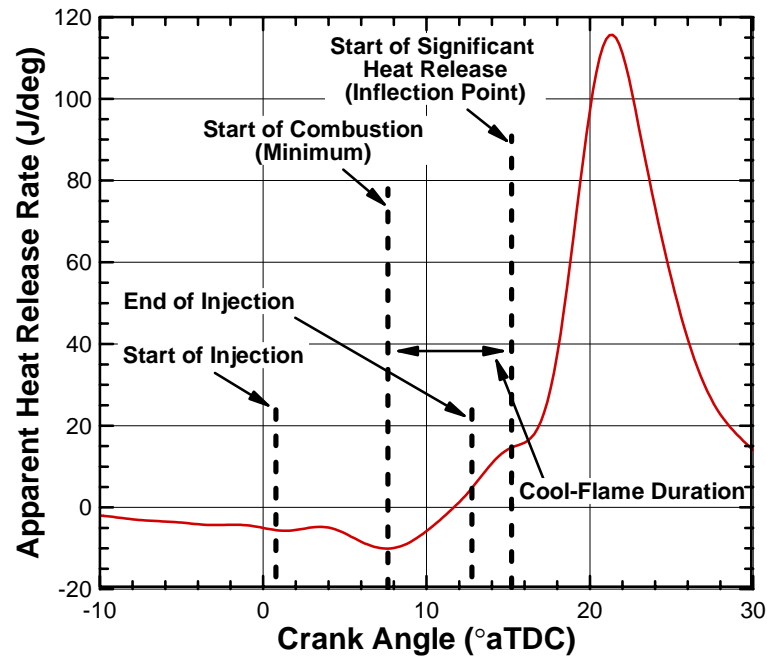


Figure 3 Apparent heat release rate as function of engine crank angle, illustrating the calculation of cool-flame duration and other locations of interest.

The equivalence ratio of the mixture at SOC is a dominant factor in the determination of the combustion path as well as the cool-flame duration estimation. Part of the work presented by Kook et al. outlines a process by which to calculate the equivalence ratio of an average fuel packet at ignition [29]. By correlating the cumulative heat release “with the fraction of O_2 needed for complete combustion... a measure of the ‘average’ equivalence ratio at ignition” can be estimated [29].

The first step is to develop the MFB profile, which is part of the heat release calculation described above, for the 0% EGR case. This serves as the reference condition for all subsequent cases with increases in EGR level. For each increase in EGR, the location of start of significant heat release is compared to the reference MFB profile. The

value of the 0% EGR MFB profile at the start of significant heat release location for the EGR of interest is noted. That noted MFB value has the same meaning as the ' q/Q_{LHV} ' axis in Figure 4. From the study by Kook et al. Figure 4 was shown to not be a function of EGR level; thus only the single curve is needed.

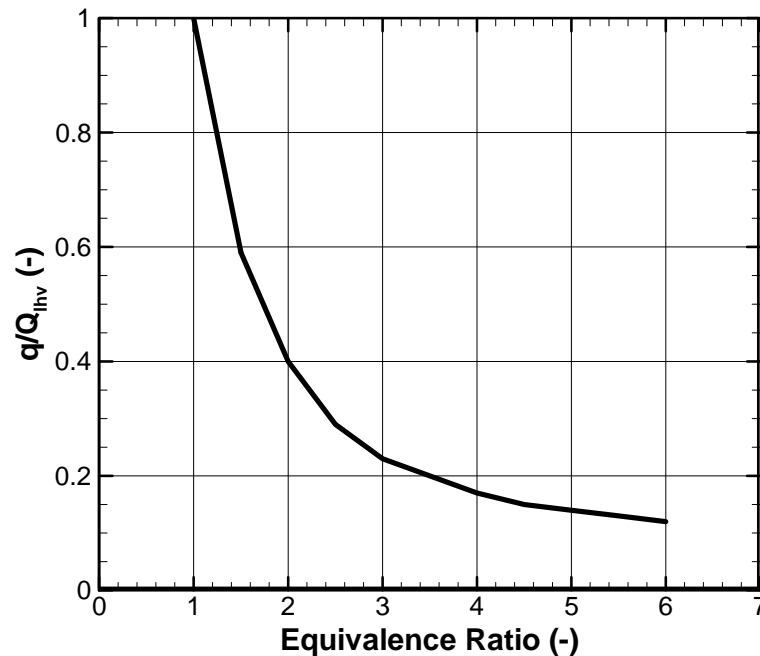


Figure 4 The fraction of energy released as a function of equivalence ratio used for hot ignition equivalence ratio calculation. Adapted from [29] which used a CHEMKIN analysis with ambient temperature of 900K This figure is the same for all EGR levels.

Figure 4 represents the results of a CHEMKIN modeling study in which the fraction of fuel energy burned as the fuel mixture becomes leaner (after injection as mixing occurs) is tracked as a function of equivalence ratio. These equivalence ratios are local values relative to an individual fuel packet, such that combustion ceases once an equivalence ratio of one is reached. The reasoning that justifies the comparison of the

reference (0% EGR) conditions to subsequent conditions with increased EGR level is the assumption that the mixing characteristics and rates are the same among EGR levels.

Thus after injection the equivalence ratio profile during mixing progression for each case should be the same. It is believed that the same assumption is applied by Kook et al. [29] Since the equivalence ratio is linked to the fuel energy consumed, by tracking this value at the specific locations the equivalence ratio for the reference condition can be determined as combustion proceeds if the MFB profile is known. Linking the increased EGR level conditions to the reference case is performed as described above.

The corresponding equivalence ratio for the input ' q/Q_{LHV} ' is finally scaled by a ratio of the stoichiometric (EGR+air)-fuel ratio at the corresponding EGR level to the stoichiometric air-fuel ratio. The difference between the two values comes from the slight change in the assumed composition of air for the EGR case. This compensates for the additional volumetric mixing that must take place in order to reach an equivalent air-fuel ratio. In order for the fuel to be mixed with the same amount of fresh air for a given amount of EGR as a case with no EGR (i.e. have the same equivalence ratio), more volume mixing must occur to reach the same mass ratio. This final value represents the hot ignition equivalence ratio for the conditions of interest.

A sample calculation is shown in the APPENDIX.

This method is implemented here to support the combustion path discussion and analysis. Although not used in the final diagnostic parameter chosen in this study, this calculation is initially targeted as such. Additionally, these values are used to explain the smoke concentration behavior observed for the late injection timing.

The results of the equivalence ratio and cool-flame duration calculations are summarized in Table 3. Data for the Conventional timing is either invalid (in the case of equivalence ratio) or not observed (in the case of cool-flame duration) and thus is not included in the table.

Table 3 Cool-flame duration and the equivalence ratio at ignition presented as a function of the EGR level at the late injection timing. Note that no cool-flame duration is observed for the conventional injection timing, nor is the equivalence ratio calculation in a valid range.

EGR Mass (%)	Equivalence Ratio at Hot ignition (-)	Cool-Flame Duration (ms)
0	Invalid ^a	0.44
15	Invalid ^a	0.65
28	Invalid ^a	0.76
42	2.2	0.93
48	2.0	1.07
53	3.1	0.90
57	4.3	0.86

^a Out of range of calculation method

2.5. Important Calculation and Measurement Summary

There are a number of important parameters that will be shown and discussed in the results and discussion sections of this study presentation. To be clear about the measurement sources and calculation methods utilized Table 4 is included. If the calculation is complex a reference to the section that describes it in detail is given.

Table 4 Measurement and Calculation methods summary listed in order of appearance.

Parameters of Interest Summary		
Parameter	Calculated or Measured	Method
EGR	Measured and Calculated	See Section 2.4.1
Heat Release Rate	Calculated	See Section 2.4.2
Mass Fraction Burned (MFB)	Calculated	See Section 2.4.2
Cool-flame duration	Calculated	See Section 2.4.3
Hot ignition Equivalence Ratio	Calculated	See Section 2.4.3
Brake Specific NO Emission	Measured and Calculated	BSNO [$\text{g}_{\text{NO}}/\text{kWh}$] = $\text{g}_{\text{NO}}/\text{Power}$
Filter Smoke Number	Measured	See Section 2.3
Cylinder Pressure	Measured	See Section 2.3
Cylinder Temperature	Calculated	See Section 2.4.2
Manifold Temperature	Measured	Using Thermocouple
CO Concentration	Measured	See Section 2.3
Combustion Duration	Calculated	Based on heat release profile
Air-Fuel Ratio	Measured	Using fuel/air flow rate values
Combustion Phasing Locations	Calculated	Based on MFB profile

3. INVESTIGATION OF THE FUNDAMENTAL MECHANISMS THAT CREATE A TWO-STAGE IGNITION EVENT

3.1. Section Objective

This first results section here presents the investigation into the fundamental explanations for the observed behavior. Specifically, the first step is to confirm the presence of a cool-flame reaction in the engine test results and that it behaves in a predictable way based on the results from [14]. With that first step as a starting point, there are two primary objectives of this study.

1. Verify the correlation in cool-flame duration between the rapid compression machine results obtained by Fish et al. [14] and the results obtained for this study. Succeeding in this, explain how changes to exhaust gas recirculation (EGR) and injection timing affect the mechanisms by which the cool-flame reaction is maintained.
2. Explain the observed correlation between cool-flame behavior and the consistent behavior in the calculated apparent heat release profile.

Subsequently explain how this behavior causes the combustion event to avoid the high soot and NO_x formation regions as described by Kamimoto and Bae [17].

A third objective is realized after completion of the two primary objectives. By correlating the cool-flame control mechanisms and the subsequent effect on the combustion event, a method for diagnosing LTC events is hypothesized. Only brief

discussion is dedicated to this goal in this section as this topic is the focus of the second results section.

3.2. Results

3.2.1. Exhaust Soot and Nitric Oxide Concentrations

The purpose of utilizing a low temperature combustion mode is to reduce both NO_x and soot concentrations. Therefore before moving into the primary purpose of this study discussion will be dedicated to showing that the desired reductions have been attained. This study utilizes a filtered smoke number (FSN), reported by the smoke meter, to give a measure of the relative concentrations of soot. The measured concentration of NO (converted to emission level) is used as an indicator of the NO_x concentration.

As an aside before continuing, some brief discussion will be given to the issue of correlations between smoke and particulate matter measurements. For this study the measured value of smoke, in units of FSN, is sufficient to make the relevant comparisons discussed. There are methods available which correlate the smoke level to a mass of particulate matter value. These correlations are empirically determined and while the smoke numbers found in this study do fall into the “valid” range of the correlation equations, the conversion has not been made in this study. The use of these correlations is a contested matter among those interested in such things, and to avoid unnecessary potential conflict the smoke number is the only value used.

For this analysis the baseline condition with which to judge measured NO and smoke values is chosen to be the 0% EGR, conventional injection timing case. The conventional timing behaves in a manner expected of a low load condition; nearly entirely premixed combustion resulting in a relatively short combustion duration. Low temperature combustion is seen as the defeat of the inverse relation between soot and NO_x. In this application (the addition of EGR) the ideal behavior is a decrease in NO without an accompanying increase in smoke that is observed in conventional combustion. The distinction is that the avoidance of an increase in soot is desired, not a reduction, as the conventional timing already achieves low smoke output. Comparing to the conventional injection timing 0% EGR case is most logical as the increased EGR and delayed injection are both control strategies used to attain the LTC mode.

The baseline established by the choice of the 0% EGR, conventional injection timing condition is a BSNO level of 8.35 g/kWh, and a smoke measurement of 0.075 FSN. As discussed above, a substantial reduction in NO and at least maintaining the baseline smoke measurement is the criteria for LTC classification. Therefore a smoke value of less than 0.075 FSN must be maintained. Based on literature review [7], a 90% reduction in NO emission is common enough that this reduction will be the targeted value used to qualify as a LTC condition. For this study an order of magnitude reduction (90%) equates to a maximum value of 0.835 g/kWh BSNO to classify as LTC. With these criteria defined, the measured values of both BSNO and smoke are shown in Figure 5. The horizontal and vertical dashed lines represent the LTC thresholds for NO and smoke respectively.

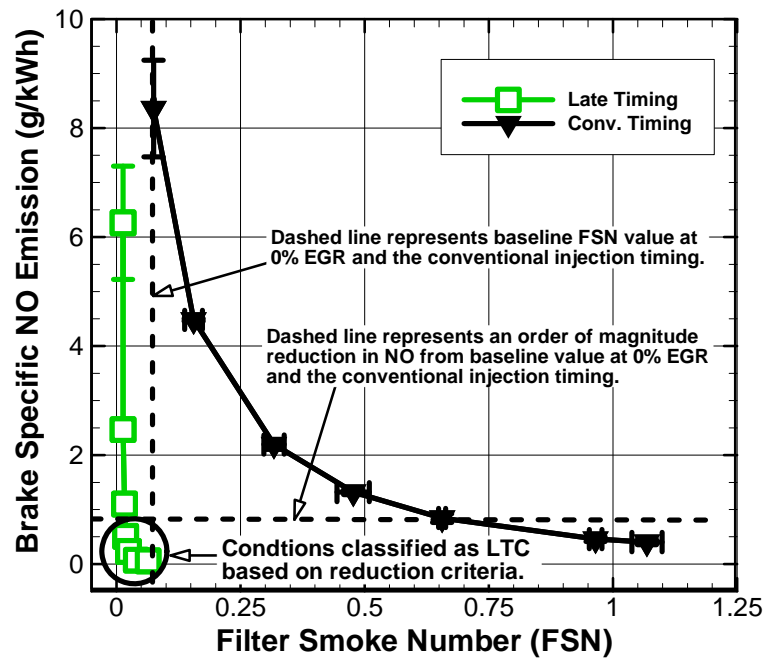


Figure 5 Nitric oxide emission (g/kW-h) versus filter smoke number as function of injection timing and EGR level.

For the conventional injection timing the typical inverse relation is observed; however, at high EGR levels for the late injection timing the smoke number also increases with a subsequent increase in EGR. This would be unexpected based on the simple definition of LTC as the defeat of the inverse relation between soot and NO_x . This behavior is attributed to the effect that equivalence ratio at hot ignition has on the “average” fuel packets combustion path. More explanation will be given, but at this point, it is most important to note simply that although the smoke measurement does increase, it still remains below the LTC classification threshold.

The emissions behavior typical of LTC has been shown. The next step is to investigate the general behavior of the cool-flame reactions, and to determine whether or

not there is a link between LTC and the presence of cool-flame. The remaining subsections of the results will perform this investigation and will explore the objectives of this study.

3.2.2. Cool-flame Properties

Verifying that a cool-flame reaction is occurring requires verification that the cool-flame duration behaves as expected. The first step in this verification is to compare the results from Fish et al. to the data collected in this study. The general trends from Fish et al.'s study [14] are as follows: 1) decreasing initial pressure increases cool-flame duration, 2) decreasing equivalence ratio increases cool-flame duration.

Figure 6 shows the calculated cool-flame duration as a function of initial pressure and the pressure at start of combustion on a log-log plot. For the rapid compression machine the data represents initial pressure and for the current engine work the data represents the pressure at start of combustion. The data from Fish et al. is represented as continuous lines for various fuels. Each line holds equivalence ratio constant and varies initial pressure and temperature; although, initial temperature had no influence [14]. The square symbols show the data of the study reported here. The equivalence ratio is not controlled, so no connecting lines are used. The important observation to make from Figure 6 is that the general trend of increasing cool-flame duration with decreasing initial pressure (or pressure at start of combustion) reported by Fish et al. [14] is apparent in the current study's work. Finally, the last thing to note on this figure is the spread observed in the data at lower pressures. This effect is linked with the equivalence ratio behavior, and will be discussed further after that data is introduced.

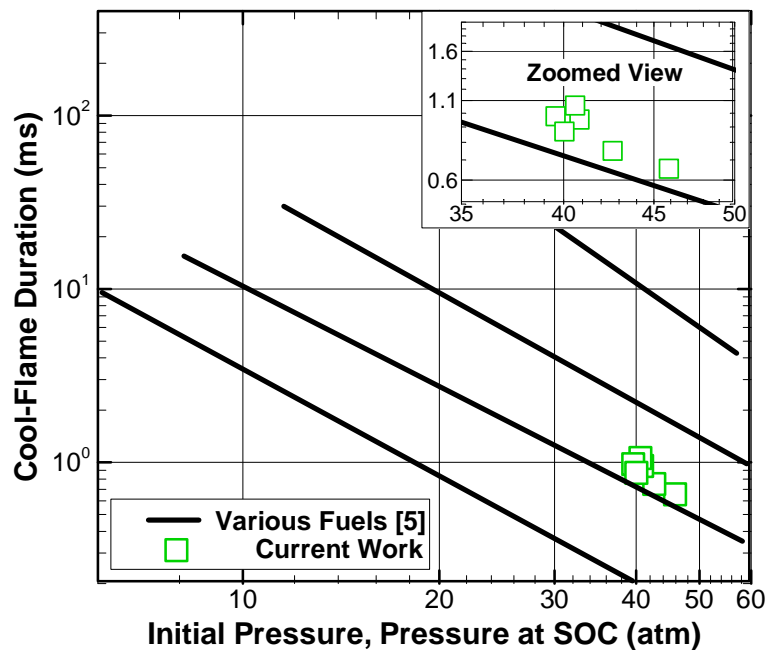


Figure 6 Cool-flame duration as a function of initial pressure from rapid compression machine experimental results (Lines) for various fuels – recreated from data shown in [14]. Engine test results from this study (Symbols) are shown as a function of the in-cylinder pressure at start of combustion (SOC). The lines represent an equivalence ratio of 0.5 with the duration not being a function of the initial temperature. Note that the equivalence ratio is not held constant for the current work; therefore a connecting line is not appropriate. Inset is zoomed view of data taken for this study – shown to make it clearer that the data does follow the same general power trend as the data from [14].

Figure 7 shows the cool-flame duration as a function of the equivalence ratio at hot ignition. These values are calculated as described in Section 2.4.3 and shown in Table 2. Fish et al. found that the duration is a strong function of equivalence ratio for lean conditions and a weak function in rich conditions. For this study, the cool-flame duration has a weak dependence on equivalence ratio in the range observed. While diesel combustion is globally lean, the heterogeneous mixture (as opposed to the homogeneous one in Fish et al.) ignites under locally rich conditions [30]. Those ignition zones control

the entire combustion event and thus the cool-flame duration in these local zones applies to the entire mixture.

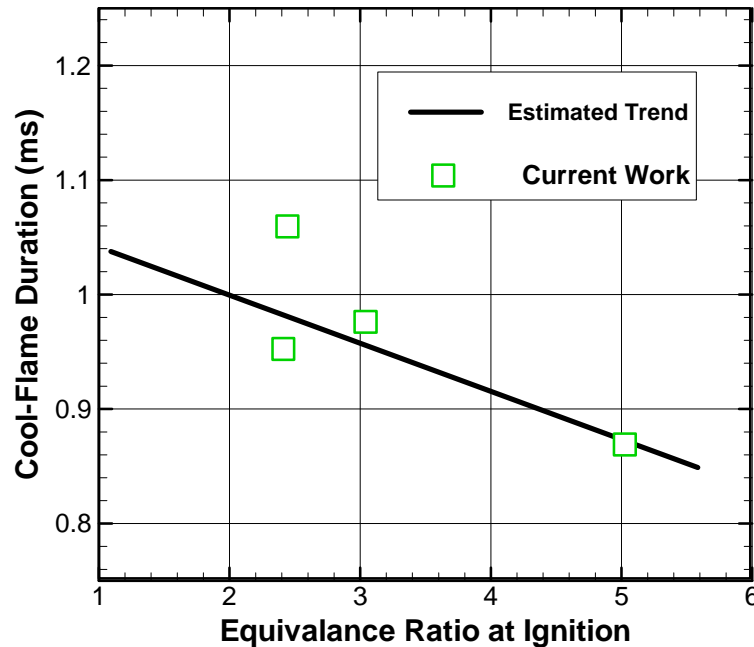


Figure 7 Cool-flame duration as a function of equivalence ratio at hot ignition. Equivalence ratio calculated by method from [29]. The estimated trend of decreasing duration with increasing equivalence ratio resembles that from [14].

Recall the observation made about the spread in data observed in Figure 6. It is believed that the behavior with equivalence ratio and initial pressure combine to produce this spread. Changes in equivalence ratio, in the range observed in this study, would change the cool-flame duration slightly even with essentially the same pressure at start of combustion. Alternatively, at a constant equivalence ratio, the cool-flame duration can change substantially with a change in initial pressure. This effect is observed for the solid lines in Figure 6. Combining these effects one can see how the general linear trend

in the log-log plot could be shifted in the vertical direction by changes in equivalence ratios. This explanation justifies the spread observed in Figure 6.

The study by Fish et al. [14] found that the cool-flame duration is a function of the initial pressure and the equivalence ratio. This study also makes this finding, matching the same general trends found by Fish et al. This correlation, between the rapid compression machine experiments performed by Fish et al. and the engine results obtained here, satisfies the first half of the first objective of this study.

This study is focused on the fundamental effect that the cool-flame reaction has on the combustion event; however, it is important to understand how and why the control parameters produce the end result. The EGR level and injection timing, the two variables controlled, combine to change the pressure at start of combustion and the equivalence ratio. While the equivalence ratio does influence the cool-flame reaction, the fact that the values are calculated estimates (rather than measured) makes the use of equivalence ratio as a predictor less attractive. Thus, since the pressure is a measured value, and its change could produce significant difference in cool-flame duration (see solid lines in Figure 6) the investigation into the influence EGR and injection timing has on the cool-flame duration will be limited to the pressure at start of combustion. Figure 8 shows the pressure at start of combustion for the two injection timings and at each EGR level. The change to the late injection timing produces a substantial drop in pressure (4-8atm) throughout the range of EGR used. The result of increasing EGR is a linear decrease in pressure across the range for both injection timings.

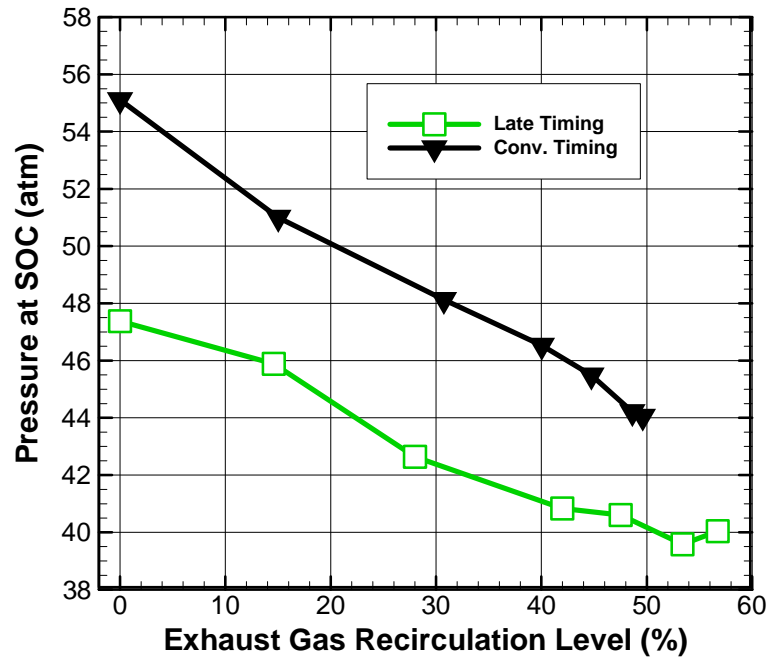


Figure 8 Pressure at start of start of combustion (SOC) as a function of EGR level and injection timing.

With the late injection occurring at TDC and the conventional timing being before TDC, it would be logical that the pressure at start of combustion would be higher for the late injection case; however, that is not the case. The difference in injection timing causes the pressure at injection to be higher for the late timing, but due to the ignition delay, the late timing combustion starts when the volume of the cylinder is larger than the conventional timing. This causes the lower pressure at start of combustion seen in Figure 8. This explanation, explaining how EGR level and injection timing affect the mechanisms by which the cool-flame reaction is maintained satisfies the second part of the first objective of this study.

A few additional comments about pressure at start of combustion. Note that the pressure for the conventional timing pressure does drop to levels comparable with low EGR levels for the late timing. It is expected then that a cool-flame reaction would be observed for those cases. However, while an inflection point is present (as described in the duration calculation method), each one occurs while the heat release rate is negative, which disqualifies it from being considered a cool-flame as described in Section 2.4.3. Also recall however that the NO drops to relatively low levels for the conventional timing, but the smoke number increases to levels similar to the baseline condition. For the conventional injection timing the inverse relation between soot and NO_x is being followed as expected.

3.2.3. Heat Release and Combustion Path

While the duration of the cool-flame reaction is an important potential indicator, the resulting effects on the whole heat release profile may be more significant. Figure 9 shows the calculated heat release profiles for all of the late injection timing cases. The general trend with increasing EGR is a decreased maximum heat release rate and longer combustion duration. Recall that cool-flame duration also increases with EGR. Figure 9(a) shows the full combustion event from slightly before injection to near end of combustion. The region shown inside the box is magnified in Figure 9(b) to highlight the effect the cool-flame reaction has on the initial stages of combustion. Increasing EGR (and cool-flame duration) does not change the start of combustion (location of minimum heat release), but the start of significant heat release location is shifted by up to nine degrees in one case. The longer combustion duration created by the correspondingly

long cool-flame reactions spreads the heat release out such that peak temperatures are minimized.

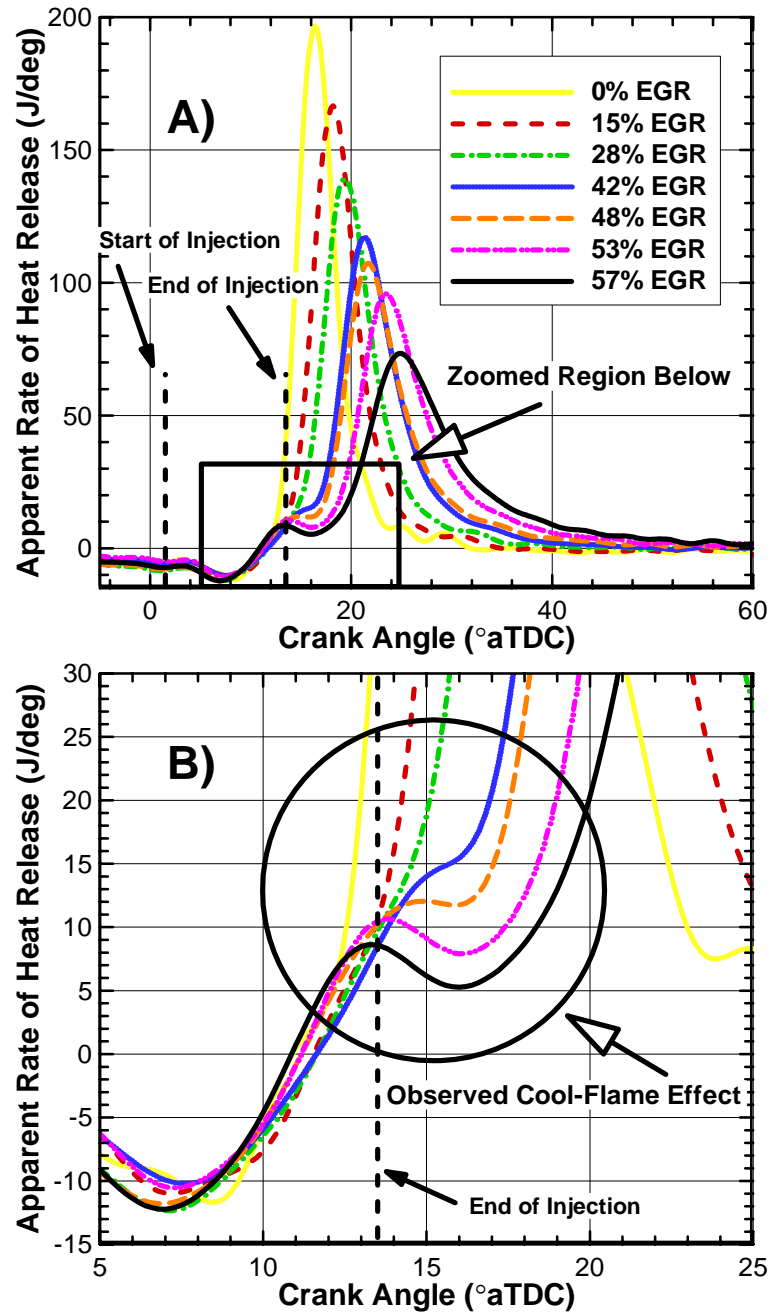


Figure 9 Apparent heat release rate for each EGR level at the late injection timing. A) Full combustion event from before injection to end of combustion. B) Zoomed view highlighting the effect the cool-flame event has on the heat release profile.

Analysis of the heat release profiles is useful in the determination of the cool-flame duration and also for highlighting the effect on the combustion event due to the presence of the cool-flame reaction. That analysis, however, does not complete the explanation of why the observed NO and FSN measurements behave as they do. The estimated combustion path will serve this purpose. Figure 10 depicts estimated conditions at start of combustion based on the equivalence ratio calculation method described in Section 2.4.3 and the calculated bulk temperature. The temperature calculation is computed during the heat release calculation process. A number of variables contribute to the path the combustion will follow as the fuel packet burns and mixes, but for this analysis the combustion paths shown are the highest possible temperatures that could be reached. This means the following assumption is used: upon hot ignition, the temperature increases during premixed reaction (constant equivalence ratio) until mixing-controlled reaction begins, at which point adiabatic flame temperature at the reaction equivalence ratio represents the reaction temperature. The author realizes that this is not what actually happens, but from the perspective of soot and NO formation, this assumption would result in maximum formation rates. No attempt is made to quantify the possible temperature differences, but the actual lower temperatures will result in lower concentrations.

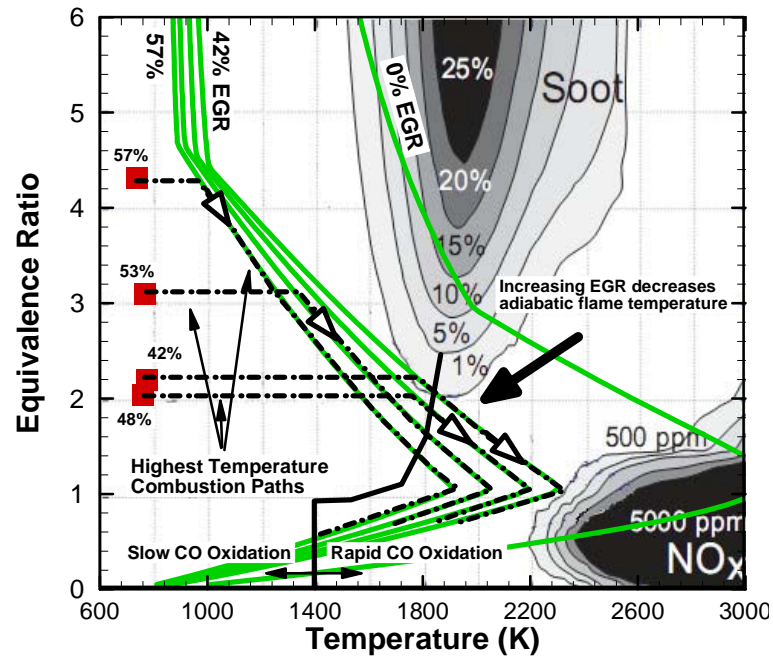


Figure 10 “Average” fuel packet combustion paths based on ignition conditions overlaid on soot and NO_x formation islands adapted from [16] based on work done by [17]. Calculated adiabatic flame temperature curves for a given EGR level represent the maximum possible temperature that could be achieved. The combustion paths shown do not represent the actual path, but only the highest possible temperatures that could be reached. The adiabatic flame temperature for 0% EGR is shown only as a reference.

It is interesting that the equivalence ratio at hot ignition increases with increasing EGR level. Recall from Section 2.4.3 the part of the equivalence ratio calculation that utilizes Figure 4 to relate MFB value to an equivalence ratio at hot ignition. The calculation method references each condition to the 0% EGR case MFB profile and the cool-flame duration (recall similar start of combustion locations from HR profiles in Figure 9) is the determining factor for the MFB value used to find the hot ignition equivalence ratio. Since the MFB profile is always increasing, longer cool-flame duration will result in a higher MFB value in the reference conditions. From Figure 4,

recall that equivalence ratio and the MFB value are inversely related. Thus longer cool-flame duration will result in a larger MFB value which produces a lower equivalence ratio at the end of the calculation. The increasing cool-flame duration is influenced by the increasing EGR which subsequently affects the MFB value at start of significant heat release. Figure 11 shows the cool-flame duration as a function of EGR level. For the points highlighted as having a valid equivalence ratio calculation output, note that the trend in cool-flame duration mirrors the trend in equivalence ratio seen in Figure 10.

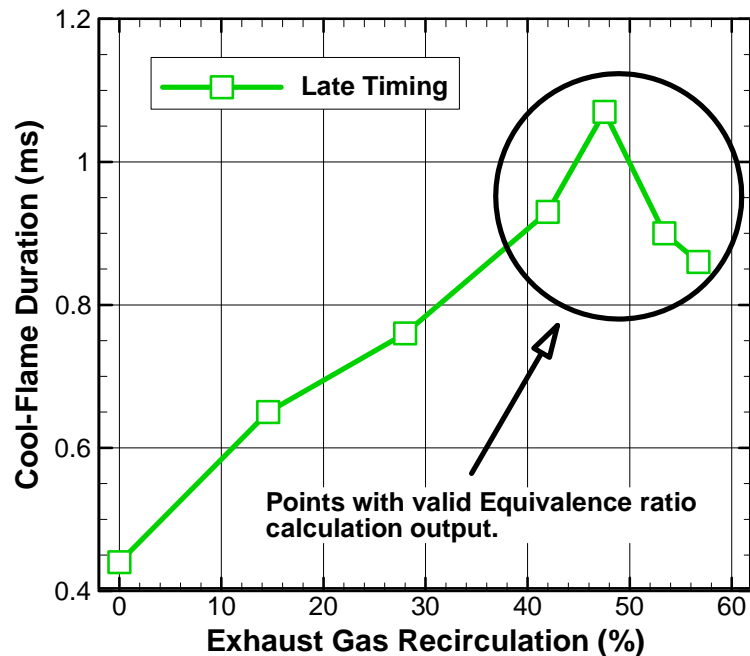


Figure 11 Cool-flame duration as a function of EGR level.

Similar to the effect equivalence ratio has on the cool-flame duration, the equivalence ratio does influence the emissions concentrations, though less so than temperature in the ranges observed in this study. The decrease in NO concentration with

increasing EGR is a result of the decreased combustion temperatures, seen in Figure 10 as the limiting adiabatic flame temperature.

Finally, note that with increasing EGR the decrease in adiabatic flame temperature moves the maximum possible temperature path closer to the boundary between slow and rapid CO oxidation. It is believed that the reduced temperature keeps the CO oxidation rate from being high enough to quickly form carbon dioxide (CO₂) despite the ample available oxygen. Figure 12 shows the CO levels as a function of EGR and injection timing. Both injection timings have high EGR levels, but the difference is the combustion duration. Recall that in the combustion path discussion, it is assumed that the combustion event followed the adiabatic flame temperature profile. For this discussion regarding the CO concentrations this assumption is not made. Consider the two injection timings with the same fuel energy being delivered (same fuel injection duration) combined with the combustion duration data shown in Figure 13. Note the longer combustion duration observed for the late injection timing at the higher EGR levels. Longer combustion duration results in a lower maximum heat release rate and thus a lower combustion temperature. Therefore despite the high EGR levels present for the conventional injection timing, there is likely substantially more time spent at temperatures that allow rapid CO oxidation to occur than the late injection timing. The large increase in CO concentrations between the injection timings supports this claim. It should be noted that this effect also plays a role in the reduction in NO formation. No further discussion is included to address this issue as this is not a primary objective of this study.

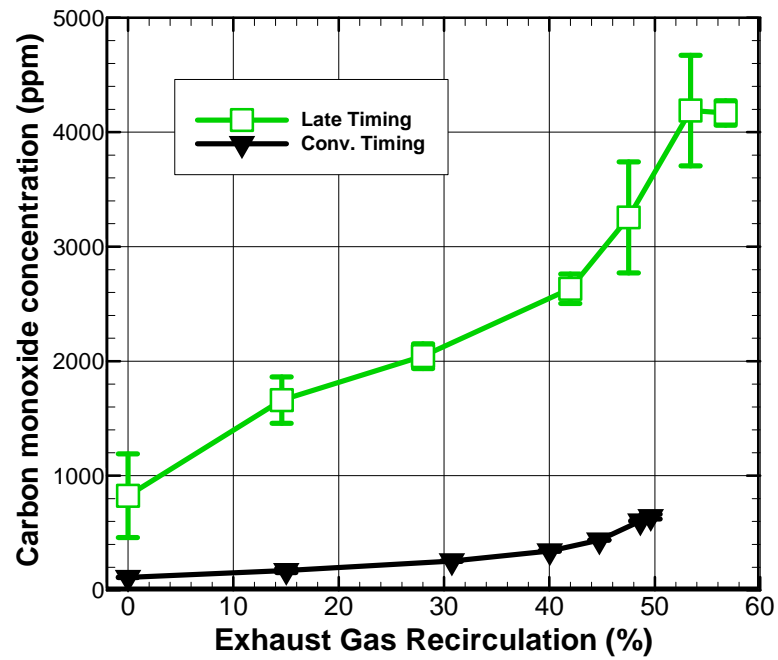


Figure 12 Carbon monoxide concentration (ppm) as a function of injection timing and EGR level.

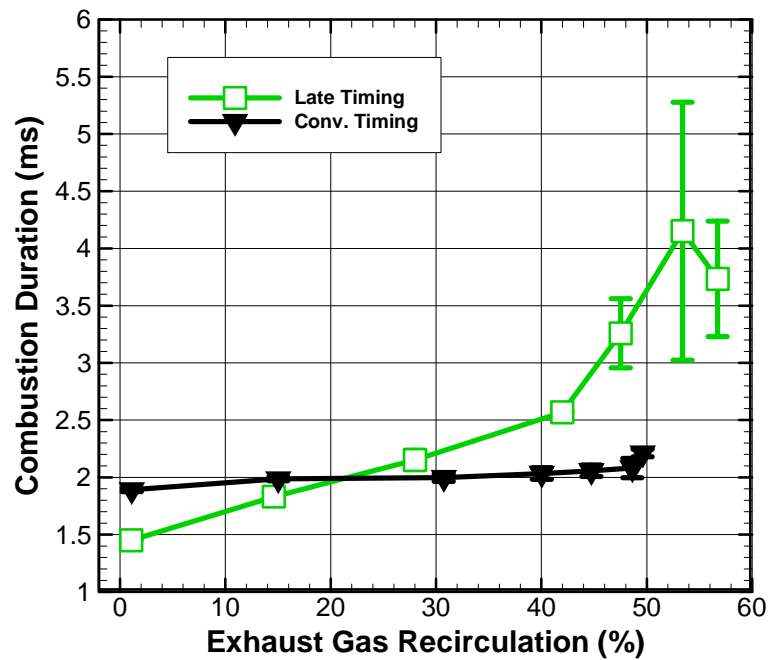


Figure 13 Combustion duration (ms) as a function of injection timing and EGR level.

3.3. Discussion

A brief discussion will be given to postulate an explanation for the observed increase in smoke as EGR is increased for the late injection timing. Also note that while increasing EGR (diluent) the combustion temperatures will decrease, the temperature of the EGR will cause the intake temperature to increase as well. This elevated temperature will cause the fuel mixture to reach hot ignition temperatures faster due to the increased temperature gradient that facilitates the heat transfer to the fuel. This results in less mixing time and thus a higher expected equivalence ratio at hot ignition. Recall that as EGR is increased the calculated equivalence ratio at hot ignition is generally increasing (see Table 3) as would be expected given this explanation. The expected (and observed) increased equivalence ratio will cause a shift into a slightly higher soot formation region seen in Figure 10. For example, combustion paths may pass through the centers of higher soot yield islands at higher equivalence ratios, thus yielding higher overall soot concentrations in spite of lower overall combustion temperatures. Although the actual illustrated soot formation regions do not extend into the region under discussion, soot formation does not simply go to zero outside the illustrated region. Although the slope of these formation regions (low temperature, high equivalence ratio) is only slightly a function of equivalence ratio, an increase in smoke would be expected to follow the increasing equivalence ratio trend.

The time dependence of soot formation could also be expected to play a role in the observed smoke measurements. The study by Kamimoto and Bae included some data that tracked soot concentration with time [17]. While the overall time scale of that data is

much longer than the combustion durations seen here, the general trend observed will likely be followed up until the concentration freeze during expansion occurs. The freeze in concentration occurs when the temperature in the cylinder drops below the level needed to promote the chemical reactions that form and break down the soot. The general trend of soot concentration with time shows increasing concentration till a peak location (reached in 15-20ms in [17]) which is followed by a decrease until the equilibrium concentration is reached. In the case of this engine study, likely the concentration will be frozen prior to reaching equilibrium (which takes 30-40 ms in [17], while combustion duration is a maximum of 4ms in this study). The peak soot concentration value and location corresponds to the peak temperature value and location respectively since the soot formation mechanism is temperature dependent. After the peak location, the concentration subsequently decreases and the soot oxidation reactions dominate the soot formation. Based on this behavior it should be expected that longer combustion duration should produce lower levels of soot (proportional to smoke measured in this study) as the oxidation mechanism operates longer. Additionally, the lower temperatures of the high EGR conditions limit the soot formation prior to oxidation such that after oxidation the engine out soot emissions are expected to decrease substantially. The factors just described highlight the potential influence of time on the expected soot formation.

All of that discussion goes to support the initial claim that increasing hot ignition equivalence ratio is the source of the slight increase in smoke number as EGR is increased at the late injection timing. The expected behavior based on time and

temperature influences is not observed, thus some other factor, such as the one postulated here, must be contributing to the results obtained in this study.

The results show that based on this study's definition of the cool-flame duration, the change in injection timing and EGR level create conditions that correlate the work done by Fish et al. with the work done in this study. The creation of the cool-flame and its subsequent duration is determined by the initial pressure and equivalence ratio. The role that injection timing and EGR level had in changing those cool-flame control mechanisms is also highlighted. Thus, the first objective of this study is satisfied – to demonstrate the correlation between this study and the work done by Fish et al. and to explain how the LTC control strategy used affects the mechanisms by which the cool-flame reaction is maintained.

The second objective of the study is to demonstrate the correlation between the cool-flame behavior and the heat release profiles and evaluate how the cool-flame reaction produces the conditions favorable for LTC. The following summary of the efforts show that this objective is satisfied. The cool-flame behavior's manifestation in the heat release profile shows increased combustion duration, and reduced peak heat release rate. Those effects, combined with the discussion about the combustion path, gives evidence that the influence of the cool-flame reaction creates conditions that cause the "average" fuel packet to follow a path that avoids the high emissions formation regions. The emissions concentrations discussion shows the attainment of substantial reduction in smoke and NO concentrations and supports the combustion path analysis. Additionally, the appearance of the inverse relation between soot and NO that appears to

be present in the LTC conditions is accounted for by the effect equivalence ratio has on the combustion path.

Combining the successful achievement of the first two objectives leads to third and final objective of this study. Under the conditions studied the cool-flame duration can be successfully and predictably influenced by the EGR level and injection timing. This result correlates the presence of a cool-flame with an observable effect on the heat release profile that can systematically be identified. Finally, the cool-flame reaction does result in the attainment of LTC, with an increasing cool-flame duration resulting in a decrease in NO and soot. Based on this supporting evidence, the author believes that a method for diagnosing an LTC condition is possible using only the heat release profile and the following section will present the results of an investigation into this theory.

4. TWO-STAGE IGNITION BEHAVIOR CHARACTERISTICS AS A LOW TEMPERATURE COMBUSTION DIAGNOSTIC TOOL

4.1. Section Objective

To develop general method of determination, independent of engine and control strategy, a fundamental understanding of the mechanisms that create a combustion event that is characterized as LTC is required. This study finds that the late injection timing and high EGR levels combine to promote conditions favorable for a two-stage ignition event. Two-stage ignition is characterized by a cool-flame reaction (slow fuel oxidation) of variable duration before start of high temperature combustion begins.

Objective. Based on a two-stage ignition and the desire for a diagnostic parameter that can be calculated from only the heat release analysis, the objective of this study is to develop and justify a set of criteria that are unique to the conditions classified as LTC based on a specified reduction requirement.

The remainder of this section will present the analysis that resulted in the chosen diagnostic criteria. Additionally, some parameters that are rejected will be shown and discussed for completeness.

4.2. Results and Discussion

The demonstration of successful LTC attainment through analysis of the measured smoke and NO concentrations is shown in Section 3.2.1 and will support the discussion in this section. To summarize the emissions results, NO measurements show that the four highest EGR levels show reductions that meet or exceed the LTC

classification criteria for the late injection timing. The same four conditions also maintain smoke measurements that fall below the LTC classification threshold. Based on this analysis, those four conditions qualify as LTC for this study. The next step is to identify a trait that sets these conditions apart from the rest. This study focuses on the two-stage ignition behavior as quantified by the cool-flame duration.

With that summary as a foundation this section is split into two sub-sections. First, an investigation into the differing effects of EGR level on the combustion event at the two injection timings under study here is shown. This is followed by the presentation of a promising method for LTC diagnostic along with some rejected methods for completeness.

4.2.1. Injection Timing and Combustion Phasing Behavior

The complexities of LTC (and engine combustion in general) are numerous – from the compounding effects of EGR and injection timing to fuel property issues (and many others), isolating a single variable is very difficult. The author here does not claim to have isolated any single variable, but in order to support the rest of the discussion a brief exploration of this particular data set and how some of these compounding issues may have been mitigated will follow in this section.

4.2.1.1. Dilution indifferences between injection timings

For both injection timings under study here there is nearly identical behavior of the air-fuel ratio with increasing EGR levels, as shown in Figure 14. The important observation to make is that simply having a highly dilute mixture is not enough to

produce a LTC condition as is evident from the NO and smoke measurements reported. Combustion phasing (manifested in this study mostly by injection timing) is crucial to the LTC attainment.

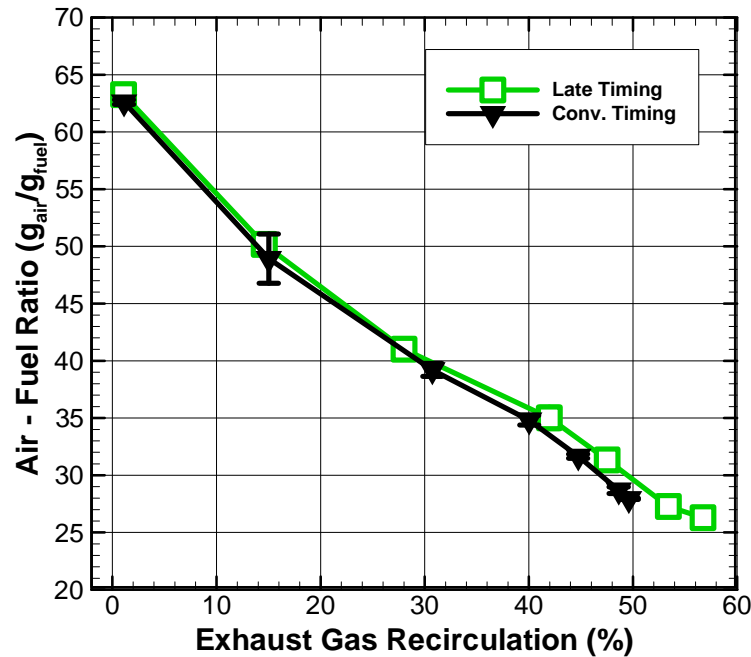


Figure 14 Air-fuel ratio as a function of injection timing and EGR level.

4.2.1.2. Combustion phasing changes with injection timing

There are some interesting characteristics of the combustion phasing that may give some insight into the effect that injection timing has despite negligible differences in dilution. Figure 15 shows the key combustion phasing parameters for all conditions under study here.

The influence of increased EGR on the combustion phasing of the conventional timing is a slight shift in start of combustion (or an increased ignition delay). However, after start of combustion, the 90% MFB and 50% MFB locations shift almost the same amount (see Figure 15A). This effect is likely why the conventional timing is not successful in achieving LTC. While the ignition is delayed, the combustion event is largely unchanged. Short combustion duration necessitates a high rate of heat release in order for the complete fuel energy to be released. This is in contrast to a longer combustion duration during which the intensity of the reaction remains low while releasing the same total energy over a longer period. Because of the nature of a piston-cylinder arrangement (neither adiabatic nor constant volume reactor) the longer combustion duration will result in lower temperatures for the same fuel delivery even if the combustion event started at the same location (which, to clarify, is not the case in this study).

For the late injection timing, the start of combustion (thus ignition delay) and 1% MFB locations are fairly steady – showing no sign of the shifting trend that is observed for the conventional timing. The 50% MFB and 90% MFB locations, however, increasingly delay as EGR is increased. Aside from the previous discussion about the advantage of longer combustion duration for producing a LTC event, the most notable thing to take from this analysis is that from the perspective of combustion phasing the cumulative heat release near ignition is not significantly affected. Additionally, because of the combustion event occurring wholly in the expansion stroke, the lower in-cylinder pressures (and thus temperatures) at start of combustion as well as the cooling effect of

expansion both greatly aid the attainment of LTC. This effect emphasizes the role combustion phasing (thus injection timing) has in LTC attainment.

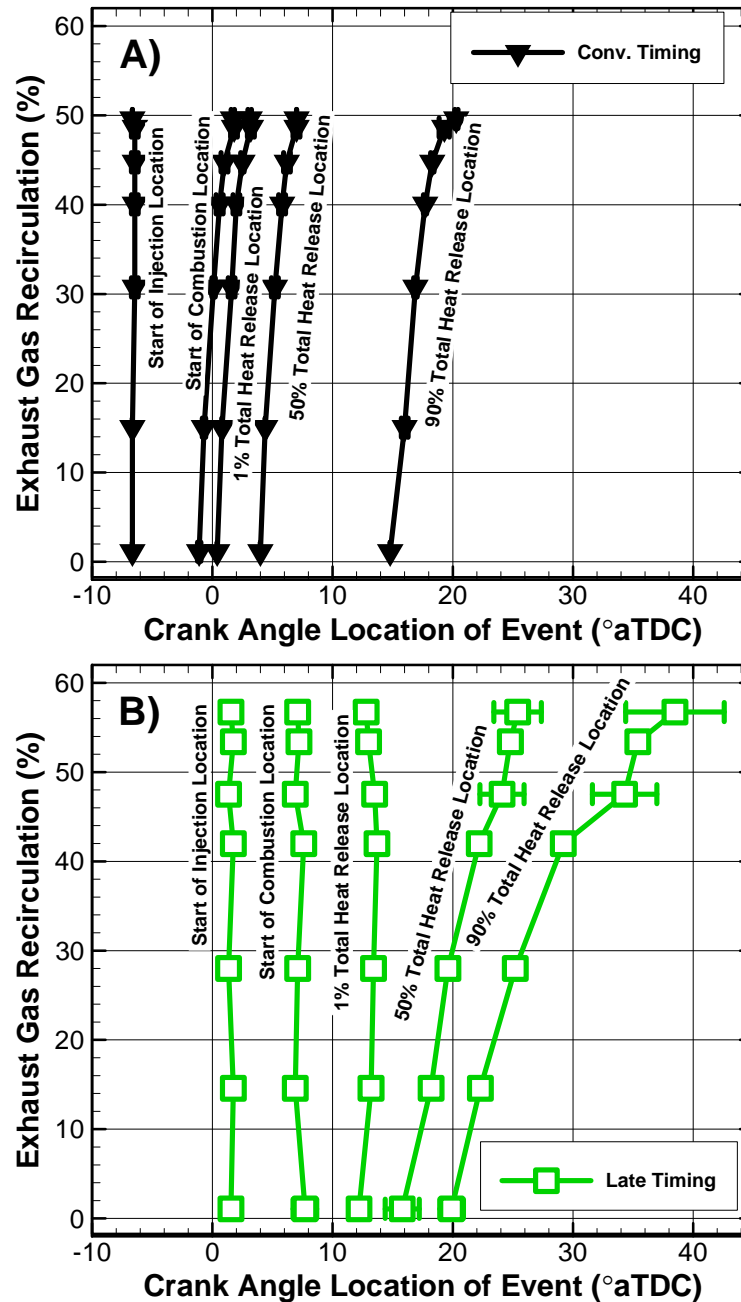


Figure 15 Combustion phasing locations as a function of EGR level for the A) conventional and B) late injection timings.

4.2.2. Low Temperature Combustion Diagnostic Method

Some further discussion about the method by which LTC is attained here for the late injection timing (and not the conventional timing) will be presented to serve as background for the diagnostic method that has been selected. The control strategies used to attain LTC typically aim to limit combustion temperatures (usually through diluents) and reduce local equivalence ratios (usually through increasing ignition delay).

For the conventional injection timing, ignition delay is affected by the addition of EGR such that ignition equivalence ratio would be expected to decrease. Similarly, the addition of EGR acting as a diluent serves to decrease the combustion temperatures. The temperature decrease is significant enough to substantially lower the NO formation, yet not enough to avoid the soot formation islands shown in Figure 10 without the combined effect of a decreasing local equivalence ratio. Clearly (based on the increasing smoke measurements with EGR) the increased ignition delay resulting from the EGR addition is not enough to attain LTC at the conventional injection timing.

In the case of late injection timing the combination of the EGR and combustion phasing create conditions that promote a two-stage ignition event. A cool-flame (slow oxidation of the fuel) reaction takes place before traditional high temperature (hot) ignition occurs. The increasing EGR lowers the pressure at ignition (a strong driving force in cool-flame reaction duration [14]) which increases the cool-flame duration such that the significant heat release is delayed long enough to phase combustion in a way that maximum combustion temperatures are limited. This limitation is created by the cooling effect as cylinder expansion proceeds in addition to the increased EGR effect on

adiabatic flame temperature. Despite the increase in local equivalence ratio (see Table 3 and Section 3.2.1), the decrease in temperature is sufficient to avoid most soot formation. The behavior of the late injection timing with increasing EGR is clear and well defined. Based on the previous discussion a criterion for diagnostic application is developed next.

4.2.2.1. The method proposed by this study

The method by which LTC is attained with conventional petroleum diesel fuel has been described briefly. With explanation to follow, the specific criteria defined here are as follows. First, a cool-flame reaction must be present. This specifically means that there is a difference in crank angle location between start of combustion and the start of the significant heat release as defined in Figure 3. Secondly, the point of start of significant heat release must occur after at least 2% of the normalized cumulative heat release has taken place. If the operating condition meets these two criteria then it shall be classified as a LTC event – see Figure 16 for illustration of these criteria.

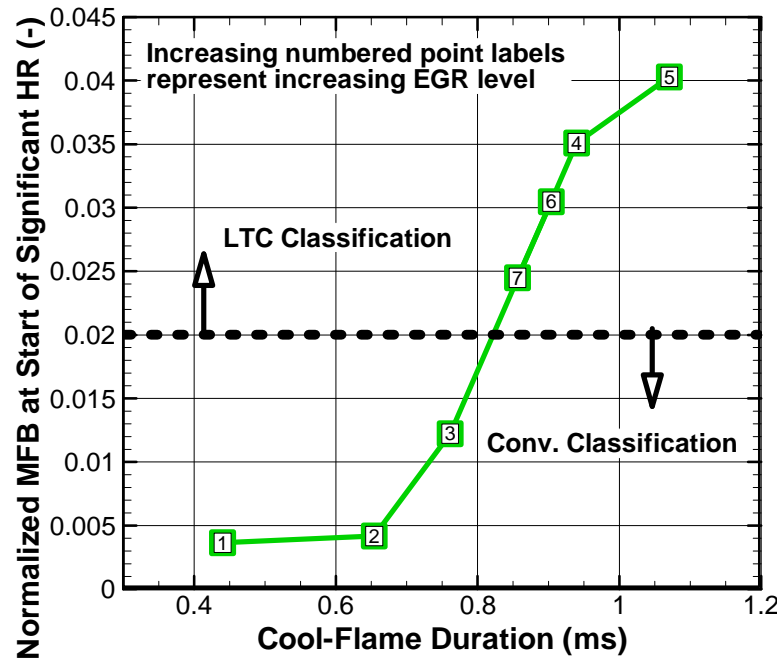


Figure 16 Normalized mass fraction burned value at the start of significant heat release location plotted against the cool-flame reaction duration.

It is postulated that under these conditions (late injection, high EGR level) the length of time required to consume 2% of the total fuel energy in a cool-flame reaction mode delays combustion such that most, if not all, fuel burns in a premixed fashion during high temperature heat release. Observing the normalized mass fraction burned profile shape in Figure 17 gives support to this claim. The slowing burn rate (the steeper the slope, the faster the burn rate) of the high EGR conditions would be indicative of a diffusion burn regime under normal compression ignition direct injection circumstances, but as indicated in Figure 17 by the vertical dashed line, the injection ends well before the slow burn behavior commences. This slow burn rate is the reason that the combustion duration increases – drastically reducing the intensity of the combustion

event and thus decreasing combustion temperatures. For contrast, the 0% EGR line shown in Figure 17 has short cool-flame duration and thus the majority of the combustion event still occurs under high temperature conditions (closer to TDC). Additionally, in the 10-90% MFB region, the burn rate is relatively fast when compared to the high EGR level conditions. Once again the importance of the combustion phasing is highlighted as being at least if not more important than a highly diluted mixture.

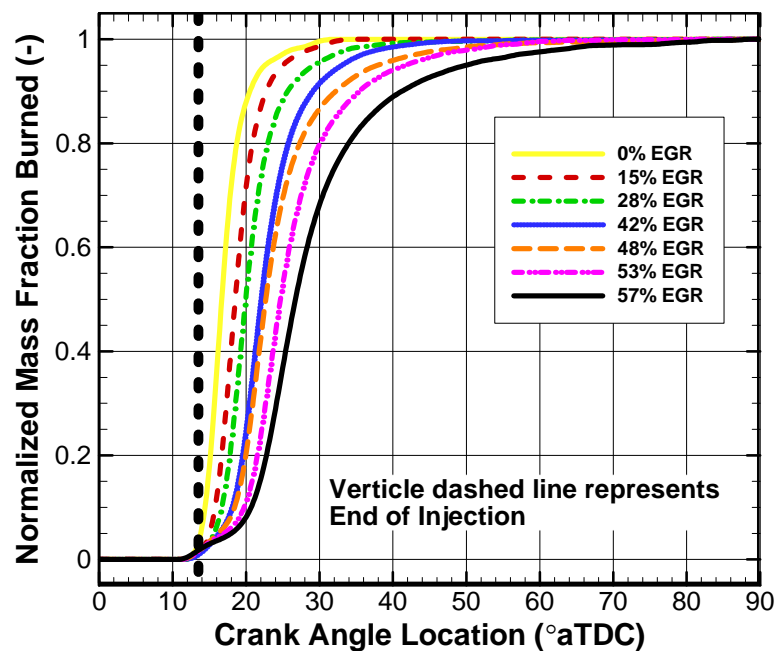


Figure 17 Normalized mass fraction burned profiles for each EGR level at the late injection timing.

It should be noted that despite the end of injection occurring prior to significant heat release, a portion of the combustion event may include some diffusion burning of liquid fuel droplets. Taking this effect into account, the behavior of the burn rate in

Figure 17 may be slightly influenced by this droplet diffusion burning. Since there is no observed transition stage from premixed burning to droplet burning, this effect likely does not play a significant role. Therefore, the slow burn rate is likely primarily a result of the cool-flame behavior described previously since the slow burn rate is present through the entire burn profile.

It should be noted that the 2% cut-off is not based on any fundamental reasoning. The effects on the heat release profile that lead to this choice, however, are based on fundamental understanding. The behavior of the cool-flame reaction and the effects that it has on the combustion event has been demonstrated and is well understood. Those effects are manifested in the calculated heat release in such a way that lends itself to this type of diagnostic parameter. Therefore as a cutoff limit in an applied control application a threshold value would need to be assigned and in this study 2% neatly includes all the points classified as LTC in Section 3.2.1. In reality a number closer to 1% might be sufficient. If applied to this study one additional test condition would have been classified as LTC. This same point achieves an 87% NO reduction while also being below the smoke number cutoff. This is all a “personal/end use” preference and in a full scale commercial application of something similar to the method discussed here would require a more detailed sweep of the possible control conditions.

4.2.2.2. Other diagnostic methods considered but rejected

Three other criteria were considered during this study – ignition pressure, cool-flame duration and hot ignition equivalence ratio. The first two only required the heat release calculation, while the third (hot ignition equivalence ratio) required some

additional information such as the stoichiometric air-fuel ratio for the EGR level used. The calculation method is much more involved, but since it is not utilized extensively in this study, the author directs those who are interested to the study by Kook et al. [29].

The use of ignition pressure as a diagnostic parameter would be the simplest method of all those investigated here. The points classified as LTC based on the discussion in Section 3.2.1 all have an ignition pressure less than 42 bar as seen in Figure 18. The justification being that a low ignition pressure would promote a long cool-flame reaction which leads to a LTC condition. Despite not being classified LTC, however, certain late injection timing conditions with cool-flames overlap those of the conventional injection timing. Hence, ignition pressure can predict, though not guarantee the presence of, a cool-flame. Yet the mere presence of a cool-flame does not guarantee LTC attainment. Therefore its use as a solitary diagnostic tool is ill advised.

Moving past the ignition pressure metric and simply using a cool-flame duration threshold is a step closer to linking a diagnostic parameter with determining LTC attainment; this metric, however, seems to require an arbitrarily-assigned cutoff value. Again, this is not advised. In this study, for example, a cool-flame duration cutoff could be 0.8ms (see Figure 18). The extreme EGR conditions, however, demonstrate a decrease in the cool-flame duration despite continued decrease in NO emissions. This complication of cool-flame behavior makes it an unfavorable for diagnostic metric.

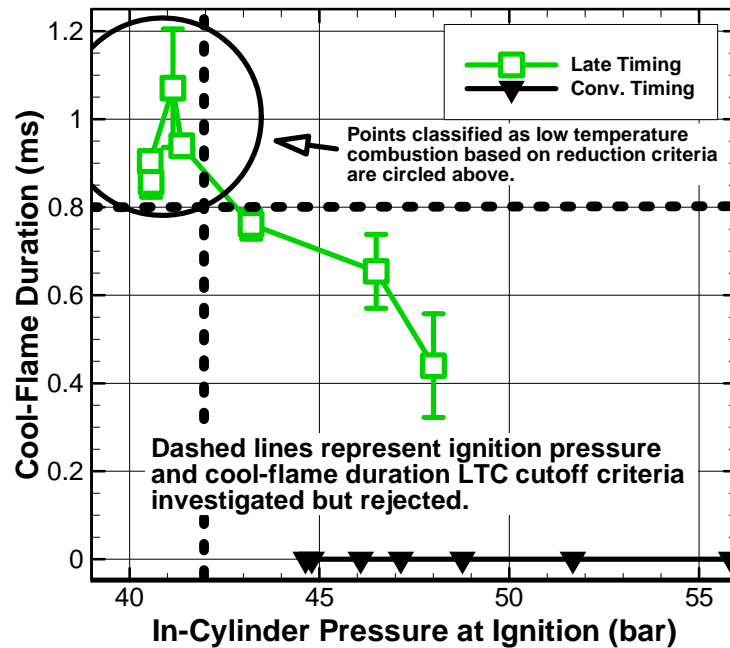


Figure 18 Cool-flame duration (ms) as a function of in-cylinder pressure at ignition (bar).

The third method involves the calculation of an estimated equivalence ratio at hot ignition for an “average” fuel packet. Only certain conditions produce a meaningful output from the calculation method. In Figure 19 the points that don’t produce a valid output are simply set to an upper threshold equivalence ratio of six. Three of the late injection timing points and all of the conventional timing points do not qualify as a valid calculation. The four points that do qualify are also the four points that are classified as LTC in Section 3.2.1. Once again no details of this calculation will be given here as the MFB threshold at start of significant heat release method discussed above is chosen due to its relative simplicity. The calculation results, however, are nearly parallel in trend and relative magnitude between both methods. A condition that qualifies under the

criteria proposed in this study will also qualify as a valid output from the hot ignition equivalence ratio calculation.

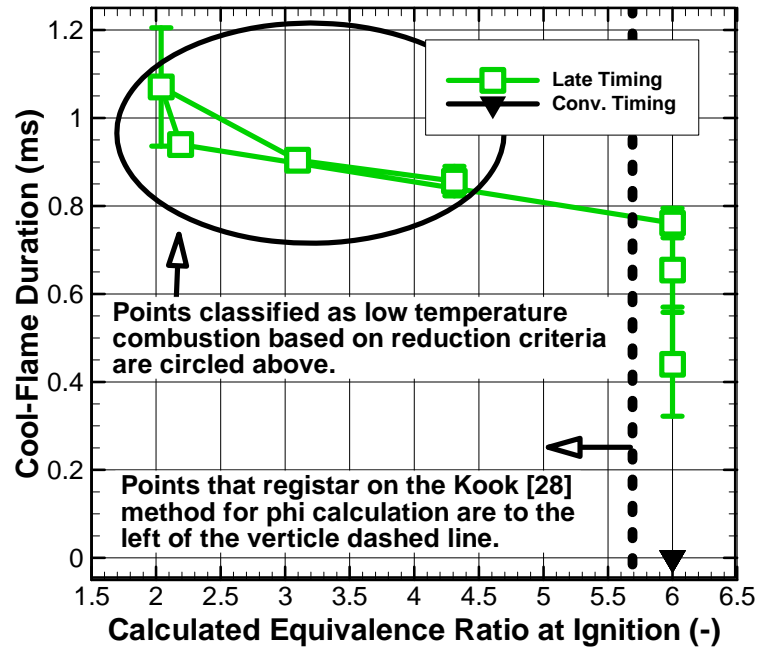


Figure 19 Cool-flame duration (ms) as a function of the calculated equivalence ratio at hot ignition.

5. SUMMARY AND CONCLUSIONS

The study done by Fish et al., which used a homogeneous mixture in a rapid compression machine, found that the correlation between cool-flame duration, pressure and equivalence ratio is valid for a number of fuels and over large ranges of initial mixture temperature and pressure [14]. Their results suggest that the cool flame characteristics determine the delay before the hot ignition commences. This study attempts to assess whether or not this result applies to a combustion event in a diesel engine. Successfully correlating the engine data cool-flame duration behavior with the study of Fish et al. suggests that there is a cool-flame reaction occurring. Therefore, the resulting changes to the heat release profile are in fact due to the cool-flame reaction. By bridging the gap between the controlled rapid compression machine experiments and the production engine there is an opportunity for using knowledge of cool-flames to predict engine behavior. The conditions that are conducive to cool-flames can be manipulated by changing the injection timing and EGR level. Applying the combustion path prediction method developed by Kook et al. it can be seen how the same conditions that promote cool-flames also result in the avoidance of the emissions formation regions [29]. Based on this correlation, if significant cool-flame behavior is observed in the heat release profile then the combustion event is believed to be in a LTC regime.

Taking the loose specification that significant cool-flame behavior indicates a LTC event, the development of specific diagnostic criteria by which LTC conditions in a medium-duty diesel engine may be identified is the next step. Currently the method

discussed here is limited in application to highly dilute late injection control strategies that undergo a two-stage ignition process.

The LTC classification criteria based on exhaust species concentrations are selected to be a 90% reduction in NO without an increase in smoke output. The baseline condition that the reduction is referenced to is conventional injection timing without EGR. The specific threshold values for this study are a BSNO level of 8.35 g/kWh, and a smoke measurement of 0.075 FSN.

There is an interesting trend for the late injection timing that shows smoke concentration increasing with increasing EGR. Although the smoke levels remain below the cutoff for LTC classification, the increasing behavior is not expected based on the traditional definition of LTC as being the defeat of the inverse relation between soot and NO_x. It is postulated that the increasing hot ignition equivalence ratio (based on calculations described in [29]) cause combustion to occur in a relatively higher soot formation island despite the low temperatures characteristic of LTC.

Based on the LTC classification requirements two diagnostic criteria are developed that identify only those points classified as LTC after the reduction criteria is applied. The specific criteria are as follows: 1. a two-stage ignition event must be present. 2. The duration of the cool-flame reaction (1st stage) must be long enough such that 2% of the normalized fuel energy is consumed before hot ignition occurs (2nd stage).

Future work will attempt to put this diagnostic method to the test of identifying LTC conditions at other control settings. One thing to consider here is that it is not likely all LTC conditions will have a two-stage ignition. It would be presumptuous to state that

this diagnostic method would encompass all LTC conditions – likely an array of tools would be needed to implement a consumer ready control system. It may be that the method presented here is applied if a cool-flame is detected, but further validation is needed and will likely be the focus of some future work.

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APPENDIX

SAMPLE IGNITION EQUIVALENCE RATIO CALCULATION

The calculation procedure here will follow the description given in Section 2.4.3. These figures are simple examples to illustrate the calculation method. Figure A-1 shows the first four steps in graphic representation. The final result is obtained by multiplying the result from Step 4 by the stoichiometric air-fuel ratio for the EGR level of interest divided by the stoichiometric air-fuel ratio of the reference condition. The stoichiometric (EGR+air)-fuel ratio for the condition of interest is 17.7 and the stoichiometric air-fuel ratio for the reference condition is 15.8. The final result is an ignition equivalence ratio of 2.46.

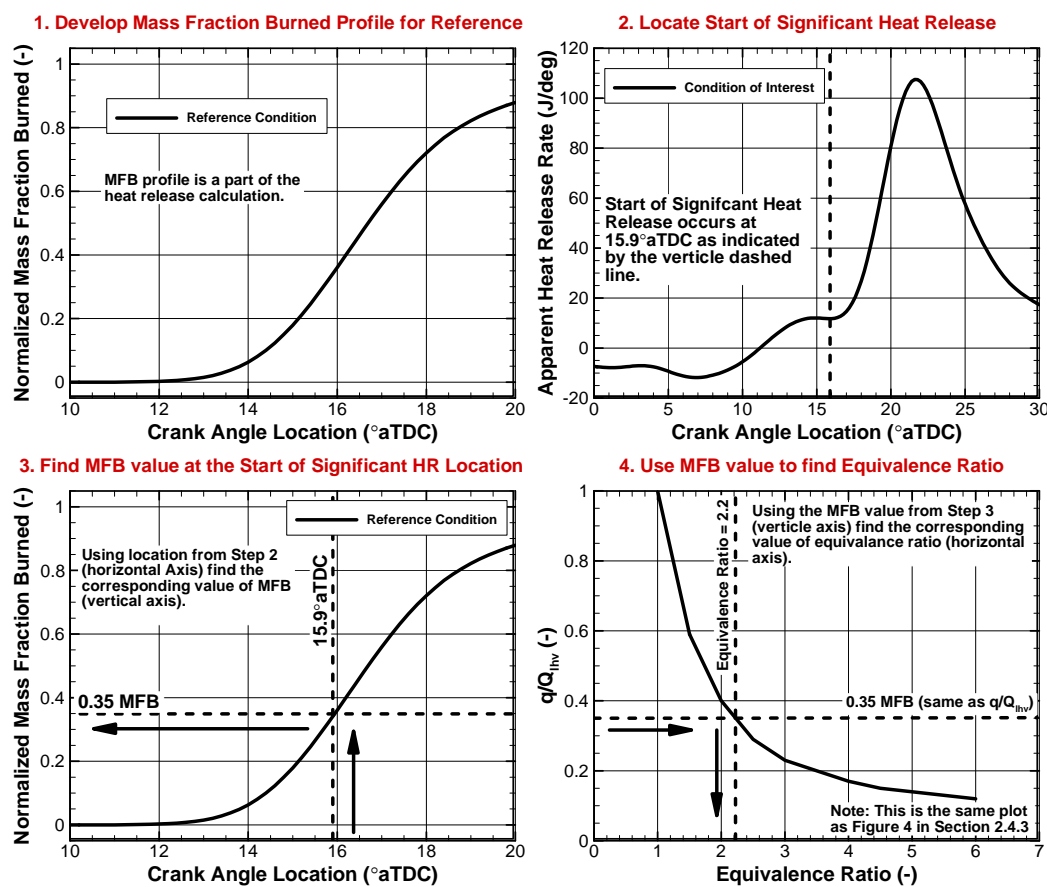


Figure A-1 Graphic illustration of ignition equivalence ratio calculation

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