On the sensitivity of low temperature combustion to spark assist near flame limit conditions

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Abstract

Spark assisted compression ignition (SACI) is a practical mode for controlling the heat release rate of low temperature combustion (LTC). While flames are key phenomena in the SACI combustion process, they may not always be effective or viable under the mildly stratified and highly dilute low burned gas temperature conditions of LTC. To better understand the limits of flammability or flame effectiveness, this work explores combustion within a single cylinder direct injection engine near the high load limit of the HCCI combustion regime, where spark induced flame propagation has been seen to affect combustion phasing and heat release rate. Flame limiting conditions were identified using progressively more advanced spark timing, up to 120° before top dead center, for differing levels of air and EGR dilution while holding the chemical energy content of the charge constant. Under air dilute conditions, the measured combustion phasing advanced from 8° to 0° after top dead center with spark advance, while almost no effect was seen under EGR dilute conditions. Estimates of the experimental global and local state conditions were made at the time of spark using heat release analysis and a KIVA-3V engine model, respectively, and the flammability for each case was evaluated using the Karlovitz criterion. The results show that fuel rich stratification near the spark plug was likely responsible for the observed variations in the SACI flame behavior.

Keywords

Homogeneous charge compression ignition (HCCI)

Spark assisted compression ignition (SACI)

Low temperature combustion (LTC)

Flame quenching

Flammability

1. Introduction

Spark assisted compression ignition (SACI) has been demonstrated as a method to control the phasing, burn rate, and stability of a primarily auto-igniting fuel/air charge [1, 2]. Optical engine studies of SACI suggest the spark event initiates flame propagation within a highly dilute mixture, accelerating the auto-ignition of the surrounding unburned charge via compression heating [3-5]. The spark provides a crucial parameter for control during transient mode switches between homogeneous charge compression ignition (HCCI), SACI, and spark ignited (SI) combustion, which may be necessary to implement low temperature combustion (LTC) in practical engines [6, 7]. Understanding the effectiveness of dilute SACI flames and their ability to control combustion phasing at a given operating condition is critical for avoiding periods of excessive pressure rise rates or instability and misfire.

While experience has shown that gasoline fueled spark ignited engines encounter a lean limit at approximately 30% dilution by mass [8], it is possible to sustain flames under higher levels of dilution provided the unburned gas temperature (T_u) is in the vicinity of the auto-ignition temperature and the energy content of the charge is sufficiently high [9]. For a given spark timing, as T_u increases conditions become more favorable for auto-ignition and flame propagation tends to become an increasingly smaller percentage of the overall heat release [2]. In practical SACI engines, T_u and dilution level are controlled by valve timing strategies that retain large quantities of high temperature residual gas, which can range from 30% to 60% of the total charge mass, depending on engine load [2].

Due to high levels of charge dilution, SACI flames have reduced burned gas temperatures (T_b) relative to undilute stoichiometric flames typical of SI engines [9]. Laminar flame simulations have predicted that premixed flames can be sustained under ultra-dilute conditions provided that T_b exceeds ~1450 to 1500 K [10-13]; otherwise, flame quenching can be induced by processes such as turbulent strain or external heat loss [14-17]. It has been proposed based upon dimensional analysis that when the flame thickness exceeds the smallest scales of the turbulent flow, transport rates within the flame are increased, broadening it to the point where there is a sharp drop in temperature that leads to flame extinction. This limit is known as the Klimov-Williams criterion [18]. However, the existence of such

behavior has not been directly confirmed; rather, flames have been observed to remain viable even when the flame thickness is many times that of the smallest scale of the turbulent flow, both experimentally and in direct simulation [16, 17, 19].

Several fundamental experiments have examined turbulent flame quenching. Abdel-Gayed et al. [20] compared schlieren images of turbulent flames from fan stirred bombs over a broad range of turbulent intensities and equivalence ratios for both hydrocarbon and hydrogen fuels to define the regimes of turbulent flame propagation. Flame appearance and quenching were well correlated to the Karlovitz (Ka) and Lewis numbers. Roberts et al. [17] used a laminar toroidal vortex to quench laminar premixed methane flames with a fuel-to-air equivalence ratio (ϕ) equal to 0.55. The maximum temperature of the product gases for the unperturbed laminar flames was 1525 K; quenching was observed to occur when the product gas temperatures cooled to ~1300 K. Quenching vortex Karlovitz numbers (~4.5-14) were similar to the two-dimensional direct numerical simulations of Poinso et al. [16]. Roberts et al. [17] also found the quenching Ka for propane-air flames differed from that of methane-air flames, indicating the importance of detailed chemistry and transport properties to the quenching process.

Additional studies have investigated flame quenching in SI engines. Quader [8] performed experiments in a single cylinder engine with adjustable compression ratio to understand if flame initiation and/or flame propagation limited lean SI operation. In the experiments, spark timing was advanced earlier into compression and away from maximum brake torque (MBT) timing to define the ignition limit where the onset of misfire occurred. Additionally, the partial burn/flame propagation limit was found by retarding spark timing from MBT until incomplete flame propagation, as determined by the lack of an ionization signal near the cylinder wall, occurred in at least 2-4% of the cycles. As the mixture was leaned, the two limits converged at the MBT lean misfire limit ($\phi = 0.65$), indicating that both ignition and flame propagation constrain highly dilute operation. Peterson et al. [21] used high-speed fuel fluorescence and particle image velocimetry measurements combined with spark discharge measurements to identify the cause of misfire and partial burn cycles in a stratified spark ignited direct injection engine. The results of the study showed abnormal spark behavior was not the cause of misfire, as all cycles had

sufficient electrical spark energy to ignite the mixture near the spark plug. For the cycles that misfired, it was shown that a flame kernel developed but failed to propagate due to the highly lean/dilute mixtures surrounding the flame kernel.

While simple models exist for the prediction of misfire, these models have not been validated under the highly dilute conditions typical of SACI/LTC. Dai et al. [15] validated a misfire model for SI combustion based on the flame quench correlations reported in the Leeds diagram of Abdel-Gayed et al. [20]. The model was implemented into a cycle simulation, which in turn determined the parameters necessary for the misfire model. With the misfire model, the cycle simulation was capable of predicting corresponding experimental misfire limits (defined when at least 0.5 to 1% of the total cycles misfired) for two engine designs using a variety of equivalence ratios, exhaust gas recirculation (EGR) rates, spark timings, and speeds and loads. For this definition of misfire, the experimental misfire limit closely matched the quenching limit of the Leeds diagram based on model predictions of turbulent flow and laminar flame characteristics at the time of spark. Dai et al. [15] predicted that this result would likely be applicable to most SI engines.

A variety of diluents can be used with LTC, and it is well known that dilution method impacts the combustion process. Dilution with EGR as opposed to air has been studied extensively in HCCI and SI combustion, including the effects on ignition delay time and laminar flame speed. Dec et al. [22] and Olsson et al. [23] showed that the use of EGR as opposed to air dilution reduced peak rates of heat release and increased combustion duration for HCCI combustion at constant phasing (CA50). Kodavasal et al. [24] used CFD modeling to compare air and EGR dilute HCCI combustion with the same ignition timing, minimal compositional stratification, and similar levels of thermal stratification. The results showed that differences in burn duration between the cases were due to variations in the mixture ratio of specific heats, which affected the work transfer between the earlier and later burning portions of the HCCI charge.

Laminar flame simulations by Middleton et al. [13] indicated laminar burning velocities decreased with increased levels of EGR dilution (versus air dilution) due to thermal and chemical effects. Flame speed was shown to be most sensitive to the high temperature chain branching and chain

terminating reaction rates which were affected by the mixture O_2 concentration. These results suggest that EGR dilute mixtures are less likely to be affected by spark assist than air dilute mixtures with the same charge energy content. It was also noted in Olesky et al. [25] that the early rates of heat release consistent with flame propagation were more rapid for air dilute SACI conditions compared with EGR dilute SACI conditions at constant fueling, spark timing, combustion phasing, and dilution level.

The sensitivity of low temperature combustion to spark assist near flame limiting conditions continues to be an area of high uncertainty and little experimental data. In the current study, a novel method is used to quantify the sensitivity of HCCI/SACI operation to spark ignition at ~4 bar (0.4 MPa) net indicated mean effective pressure ($IMEP_n$), a load condition where flames have been shown to have an influence on the timing and rate of combustion [26, 27]. (At loads less than 3 bar $IMEP_n$, almost no spark effect has been seen as the mixture is very dilute [26-28]). The experiments presented here, performed on a single cylinder metal engine with a gasoline direct injection fuel system, studied the effects of air/EGR dilution and spark timing on combustion phasing while holding the chemical energy content of the charge constant. Detailed analysis of the experimental results was performed to understand the processes governing the observed SACI heat release rates and to provide insight into proposed flame limiting behaviors.

2. Experimental apparatus and methods

2.1 Research engine

Experiments were performed with a single cylinder gasoline direct injection research engine. Key geometric parameters are listed in Table 1, with a complete description of the experimental facility provided in a previous publication [2]. The four valve engine is equipped with a fully flexible valve actuation system, allowing for independent control of valve lift and duration. With this system, a large amount of internal EGR was retained using symmetric negative valve overlap (NVO) in which the early closing of the exhaust valve during the exhaust stroke trapped hot residual gases in the cylinder to initiate combustion in the following cycle. An external EGR loop with a water-cooled heat exchanger allowed

cooled EGR gases to be introduced to the intake manifold, where electric heaters controlled the temperature of the incoming charge. Gasoline with an anti-knock index (AKI, i.e. the mean of the research and motor octane numbers) of 87 was delivered from a solenoid fuel injector mounted between the two intake valves during the early part of the intake stroke (during NVO) at 330° before top dead center (bTDC) of combustion. A spark plug with a gap of 0.9 mm was mounted in the center of the cylinder head. The rated energy delivered from the spark plug coil (~70 mJ) was held constant throughout the experiment.

2.2 Data acquisition and combustion analysis

Cylinder pressure data was sampled at 0.1° crank angle (CA) resolution for 200 consecutive cycles using a piezoelectric pressure transducer (Kistler 6125A). Pressure dynamics in the intake and exhaust runners were recorded at the same resolution using piezoresistive transducers (Kistler 4007 and 4045, respectively) mounted near the ports. A wideband oxygen sensor (ETAS LA4) in the exhaust manifold was used to determine the fuel-to-air equivalence ratio (ϕ), while exhaust constituents (CO₂, O₂, CO, THC, and NO_x) were measured with an emissions analysis system (Horiba MEXA-7100DEGR). The oxygen molar fraction in the unburned charge was estimated by assuming that the EGR (both internal and external) was composed of products of complete combustion (CO₂, H₂O, O₂, and N₂) at the measured ϕ .

The internal residual fraction, defined as the mass remaining in the cylinder from the previous cycle relative to the total mass of the trapped charge (including fuel, air, external EGR, and internal residual gases), was estimated for each cycle using the method of Fitzgerald et al. [29]. With this method, a maximum uncertainty of $\pm 5\%$ in the measured cylinder pressure at intake valve closing (IVC) corresponds to a $\pm 2\text{-}3\%$ uncertainty in the residual gas fraction and an associated average cylinder temperature uncertainty of ± 30 K near TDC. This uncertainty is largely expected to be systematic and not affect the observed experimental trends. Additional uncertainties of key experimental measurements

include $\pm 1\%$ for peak cylinder pressure, $\pm 2\%$ for engine-out NO_x emissions, and $\pm 0.2\%$ for fuel mass flow rate.

A two-zone heat release analysis was used to estimate residual fractions, in-cylinder temperatures, and combustion rates. Details of the analysis as well as validation results can be referenced in Ortiz-Soto et al. [30]. For each cycle, a modified Woschni heat transfer correlation [31] with variable mixture properties was used to calculate the gross rate of heat release and cumulative gross heat release. From these results, combustion parameters such as phasing (CA50) and ringing intensity were calculated on a cyclic basis. Average values of these and other parameters over the 200 recorded cycles were then calculated. Ringing intensity, defined by Eng [32], was limited to an average of less than 5.0 MW/m^2 , while the coefficient of variation (CoV) of IMEP_n was less than 3% when setting the baseline HCCI conditions, discussed in Section 2.4.

2.3 Modeling framework

To support the experimental analysis, simulations were conducted with the 3-D CFD code KIVA-3V [33]. The KIVA-CFMZ model formulation chosen has been discussed in detail elsewhere [34, 35]; it simulates turbulent flame propagation using the Coherent Flamelet model (CF) [36, 37], while detailed chemistry is simulated using the fully coupled Multi-Zone approach (MZ) [38]. This model has been tuned to accurately reproduce the experimentally measured cylinder pressure data from the current engine for a variety of SI, HCCI, and SACI operating conditions and has been validated by Middleton et al. [34, 35].

Open cycle simulations were conducted with the KIVA-CFMZ model using a 156,000 cell detailed 3-D mesh with moving valves and piston corresponding to the geometry of the metal engine used in this study. A visual representation of the mesh is shown in Figure 1. The KIVA simulations were configured to match the experimental operating conditions of interest and were initialized at 640° bTDC of combustion, during the expansion stroke of the previous engine cycle, using estimates of the thermodynamic state and composition from heat release analysis [30]. Boundary conditions in the intake

and exhaust manifolds were imposed from the high speed manifold pressure measurements of the experiments. For this work, the simulations were non-reacting and were performed up to the time of spark to investigate flows and thermodynamic properties in the vicinity of the spark plug.

Flow turbulence was modeled using the standard $k-\varepsilon$ formulation for RANS, which reports the statistical mean turbulence values but is incapable of capturing stochastic scalar fluctuations within the domain that may result in cyclic variability. The initial turbulent flow field was imposed from a motored simulation of a complete 720° CA engine cycle. Fuel injection was modeled using the high-pressure swirl injector model of Chrysos [39], which accounts for both the primary and secondary atomization of fuel as well as the transition of the initial pre-swirl spray with a solid cone to the steady state behavior of the main injection event with a hollow-cone structure. The injector model has previously been validated and showed good agreement with experimental PLIF (planar laser-induced fluorescence) measurements in an optical engine [40].

2.4 Experimental procedure

The current study investigates the response of an otherwise auto-igniting mixture to spark ignition. For all experiments, the fueling rate was held constant at 12.5 mg/cycle, resulting in an approximately constant load of ~4 bar (0.4 MPa) IMEP_n at an engine speed of 2000 rpm. Three HCCI operating conditions at varying ratios of air to EGR dilution were established as baseline conditions without using spark assist. To increase the potential sensitivity to spark timing, the conditions were selected near the high load limit of the HCCI combustion regime [9] with the fuel-to-charge equivalence ratio (ϕ') held constant at $\phi' \approx 0.38$. The definition of ϕ' is given in Eq. 1 as

$$\phi' \equiv \frac{F/(A + EGR)}{(F/A)_{ST}} = \frac{\phi(1 - EGR)}{[1 + \phi \cdot EGR \cdot (F/A)_{ST}]} \cong \phi(1 - EGR) \quad (1)$$

where the masses of fuel, air, and residual gas are denoted by F , A , and EGR respectively. Here, ϕ is the fuel-to-air equivalence ratio, the subscript ST denotes stoichiometric conditions, and EGR is the total in-cylinder residual gas fraction, which can include both internal and external EGR. The approximation

holds because the stoichiometric fuel-air ratio for gasoline is ~ 0.07 , resulting in a denominator close to 1. Essentially, ϕ' is a measure of the dilution level of the charge by air and EGR and approximates engine load (relative to full load) for unthrottled naturally-aspirated dilute operating conditions [9].

The three baseline HCCI experiments were performed with the fixed engine parameters listed in Table 2. The first experiment (Case 1), shown in Table 3, used no external EGR. The intake air temperature was held constant at 45°C , and the NVO was set to 152°CA to obtain a thermal environment in which combustion phasing (CA50) occurred at $\sim 8^\circ$ after top dead center (aTDC). This combustion phasing was chosen to provide near maximum thermal efficiency for HCCI combustion [41]. Case 1 had a total dilution level of $\sim 63\%$ by mass (40% from internal residual and the remaining 23% from excess air), corresponding to $\phi = 0.62$ and an estimated O_2 molar fraction of 15.6% in the unburned mixture. The engine was operated unthrottled at this condition with the exhaust pressure 5 kPa above the intake pressure. Throughout the experiments, the valve timings were held constant to minimize the impact of flow and mixing variations associated with varying NVO on the results [42].

Two additional HCCI experiments were performed with increasing levels of external EGR. For Cases 2 and 3, shown in Table 3, external EGR was incorporated into the incoming diluent mixture while holding the total charge mass (fuel + air + EGR) constant. As external EGR was added, a portion of the incoming air was replaced with products of combustion, decreasing the in-cylinder O_2 concentration. To compensate for the resulting changes in the end of compression temperature caused by a decreasing specific heat ratio and to maintain CA50 at $\sim 8^\circ\text{aTDC}$, the intake charge temperature was increased with increasing external EGR. The intake and exhaust pressures were also increased by up to 8 kPa (0.08 bar) to maintain total charge mass by offsetting small changes in the incoming charge density. The increase in exhaust pressure was estimated to cause a 3% absolute increase in the internal residual fraction relative to Case 1. With this procedure, the cylinder pressures prior to combustion differed by less than 2% between the three Cases.

Case 3 used the highest level of external EGR, the lowest level of excess air, and the highest intake temperature and intake pressure, corresponding to $\phi = 0.97$. Case 2 used intermediate settings to

Cases 1 and 3. The three Cases were phased similarly, yet the 10% to 90% mass fraction burn duration increased by 2.3° CA (27%) with the addition of external EGR, leading to a ~40% decrease in ringing intensity and a ~50% increase in CoV of IMEP_n (shown in Table 3), similar to results from previous HCCI studies [22, 25].

Once the baseline HCCI Cases were established, spark timing was applied at 30° bTDC and then advanced in increments of 10° CA for all three Cases, continuing to 120° bTDC for Case 1. The combustion phasing was not optimized for these experiments, as the goal was to investigate the differences in combustion response behavior between the HCCI and SACI modes of operation. With this procedure, the sensitivity of combustion characteristics (e.g. CA50) to variations in spark advance was quantified and the effects of flame propagation on heat release behavior were deduced. If flames were ineffective and auto-ignition prevailed, the combustion continued to exhibit the baseline HCCI phasing ($\sim 8^\circ$ after TDC) over the range of spark timings. This method differed from previous SI engine studies that relied on incomplete combustion or partial misfire to determine flame limits [8, 15, 21] and allowed for the investigation of flame behavior at ultra-dilute operating conditions.

3. Results and discussion

3.1 Effects of spark advance on mean and cyclic combustion behavior

Figure 2 shows the CA50 response of each cycle of the baseline HCCI Cases to spark advance. The diamond symbols represent the mean of 200 consecutive cycles, while each “x” is the CA50 measurement for a given cycle. The baseline HCCI Cases (where no spark was used) are presented for reference, labeled with a spark timing of 0° aTDC. The dashed horizontal lines represent the ± 2 standard deviation (σ) spread in CA50 for the baseline HCCI Cases.

While previous experimental studies showed SACI combustion phasing to advance with advancing spark [1, 2, 5], Figure 2 shows that the mean phasing is not affected for every Case and spark timing. The most air dilute Case 1 shows the most sensitivity to spark assist, with a continuous advance in the mean combustion phasing up to a spark timing of 90° bTDC before returning to the initial HCCI

phasing at a spark advance of 120° bTDC. The mean CA50 of Case 2 shows a weak response to spark advance before returning to the initial phasing at a spark timing of 70° bTDC. The most EGR dilute Case 3 shows no significant change in mean CA50 from the HCCI phasing as spark advances. Additionally, the distributions in CA50 vary considerably among the conditions in Fig. 2. The Case 3 conditions, for example, have a similar CA50 distribution to the HCCI conditions, while the Case 1 conditions show a dramatically increased CA50 distribution as the mean CA50 advances with spark timing.

Figure 3 provides histograms of the distributions in CA50 for each condition presented in Fig. 2. For the Case 1 conditions (Fig. 3a), the increased cyclic variation in CA50 with spark advance is quite noticeable; not only does the mean CA50 advance with spark, but the spread in the CA50 distribution increases substantially. Even for the most advanced spark timing case at 120° bTDC, where the average CA50 has returned to the initial HCCI phasing, several cycles still occur with very early CA50 timing. For Case 2 (Fig. 3b), the mean CA50 advances moderately with spark advance up to 60° bTDC and the distribution widens; however, as the spark is advanced to the earliest timings, the distribution becomes more HCCI-like. For the Case 3 conditions (Fig. 3c), the mean CA50 and the distributions of CA50 do not vary noticeably as the spark is advanced, indicating that the combustion process remains HCCI-like even with spark ignition.

The cyclic variation in CA50 and combustion behavior for a given condition is further evident in Figure 4, which compares the heat release profiles of three individual cycles (out of 200) for Case 1 at a spark advance of 90° bTDC. The data are from the cycles with the most advanced CA50, the most retarded CA50, and the CA50 that falls closest to the mean value from the 200 recorded cycles. The difference in CA50 between the most advanced cycle and the most retarded cycle is $\sim 18^\circ$ CA. The heat release profile of the latest cycle resembles that of HCCI combustion, indicating that flame propagation potentially failed or was ineffective. In contrast, the most advanced cycle clearly demonstrates a significant portion of gradual heat release prior to auto-ignition, consistent with flame propagation and previous observations of SACI [1-3].

For each cycle of the Case 1 conditions, the fraction of mass consumed by flame propagation was estimated using the point of maximum positive curvature in the heat release rate (indicated in Fig. 4). The maximum curvature was calculated using the first and second derivatives of the heat release rate and has been used in previous studies [25, 30, 43] to define the transition point between flame propagation and auto-ignition in SACI combustion. It is assumed that the transition is instantaneous, and SACI combustion modeling [12] and SACI optical engine experiments [3, 4] have indicated that this is a reasonable approximation.

Figure 5 shows the fraction of flame-based heat release as a function of combustion phasing for each cycle of the Case 1 conditions in Fig. 3a. The dotted lines in each plot of Fig. 5 represent the range in the fraction of flame consumption (~4-10%) that was estimated for the 200 cycles of HCCI data, even though no flames were present. This range is the result of using the maximum curvature in the heat release rate to signal the start of auto-ignition, which for HCCI is associated with intermediate temperature heat release prior to thermal runaway [44]. For cycles with flame consumption levels at or below 10%, the overall heat release resembles that of HCCI, and it is difficult to assess whether or not flames are present. Therefore, there is uncertainty in the nature of the combustion process for flame consumption levels below this threshold. Beyond this level however, it is clear in Fig. 5 that combustion phasing is proportional to the estimated fraction of flame-based heat release. This observation is consistent with the conceptual model that spark-initiated flames further compress the surrounding unburned mixture, thereby advancing the timing of auto-ignition and CA50. While not shown in Fig. 5, similar trend-wise behavior was seen for the Case 2 and Case 3 conditions, but with much lower peak fractions of flame-based heat release. Case 2 conditions up to spark timings of 80° bTDC exhibited multiple cycles of increased flame-based heat release (compared to HCCI), while Case 3 conditions exhibited HCCI-like fractions for all spark timings.

Figure 6 provides additional insight into the combustion variability and its effects. Figure 6a shows CoV of IMEP_n as a function of spark timing for every case, while Figure 6b shows the corresponding NO_x emissions. For Case 1 conditions at spark timings up to 60° bTDC, Figure 6a

indicates that the CoV of IMEP_n is marginally affected by the increased spread in both CA50 and the fraction of flame-based heat release noted in Fig. 5. As the spark advances from 70° to 105° bTDC for the Case 1 conditions, the spread in CA50 and the fraction of flame-based heat release continue to increase, and the CoV of IMEP_n increases noticeably. For even earlier spark timings at 115° and 120° bTDC, the maximum fraction of flame-based heat release in Fig. 5 remains high; however, the number of combustion events with high levels of flame-based heat release decreases, the CA50 distribution becomes more HCCI-like, and the CoV of IMEP_n decreases. Figure 6a indicates that for highly dilute mixtures near the flammability limit, spark assist does not always increase combustion stability. This result differs from previous studies which showed that spark assist consistently improved the stability of HCCI combustion [1, 5].

The effect on NO_x of the increased fraction of flame-based heat release with combustion advance is shown in Figure 6b. For the Case 1 conditions, the NO_x emissions increase notably as spark is advanced from TDC, with the maximum NO_x emissions observed at a spark advance of 105° bTDC. The increase in NO_x is attributed to increased combustion temperatures which can occur due to two mechanisms. Since flame propagation is inherently slower than auto-ignition, the burned gas within the flame is expected to reside at elevated temperatures for longer periods of time, especially when those flames are initiated earlier in the cycle. Additionally, the increased NO_x emissions could be associated with increased peak mean gas temperatures resulting from more advanced combustion. As the Case 1 conditions become more HCCI-like at spark timings earlier than 105° bTDC, the NO_x emissions decrease to their initial values.

3.2 Estimating thermodynamic properties and flame speeds

There are two probable scenarios for the conditions that show little response to spark timing: (1) The spark-initiated flames are quenched shortly after spark, or (2) flames can be successfully initiated and propagate, but the flames do not have sufficient time to noticeably impact combustion phasing or heat

release rate prior to auto-ignition. The goal of the following analysis is to determine the likelihood of either scenario for each operating condition in order to explain the observed experimental behavior.

First, the mean global thermodynamic and compositional states of each mixture at the time of spark ignition were estimated from heat release analysis. The global compositional states are listed in Table 3, and the results for the mean unburned gas temperature (T_u) at the time of spark are presented in Figure 7a, which show that T_u decreases by ~ 300 K as spark timing advances from 30° bTDC to over 100° bTDC. The lower temperatures associated with spark advance would potentially increase the difficulty of initiating a flame. On the other hand, the lower T_u would lead to longer end-gas ignition delay times, which would allow more time for flame propagation to occur prior to auto-ignition. The most EGR dilute Case (Case 3) exhibits consistently higher T_u 's (by 20-30 K) for a given spark timing, which resulted from the increased intake temperature necessary to maintain constant HCCI combustion phasing at this equivalence ratio.

The estimated mean global unburned mixture properties and the measured cylinder pressures at the time of spark were used to estimate the corresponding burned gas temperature (T_b), laminar flame speed (S_L), and laminar flame thickness (δ) using the correlation of Middleton et al. [13], which was developed from laminar flame simulations that were validated with experimental flame data covering a broad range of pressure, unburned gas temperature, and equivalence ratio conditions for air and EGR dilute mixtures [10, 13]. Although the correlation was developed from iso-octane laminar flame predictions, the results are expected to be similar for gasoline given the comparable laminar burning velocities and ignition delay times of the two fuels [45, 46].

Estimates of T_b and S_L using the global mixture properties at the time of spark are presented in Figures 7b and 7c, respectively. As spark advances the global T_b shows a decreasing trend similar to the global T_u in Fig. 7a. Despite having higher T_u 's at the time of spark, the more EGR dilute Case 3 conditions have the lowest T_b 's (by ~ 70 K) due to the increased mixture heat capacity. The estimated global T_b 's for Cases 1 and 2 are closer in magnitude. The global S_L results in Fig. 7c show that for a given spark timing, the EGR dilute Case 3 conditions have the lowest predicted S_L while the more air

dilute Case 1 conditions have the highest predicted S_L . The results may explain why Case 1 showed the greatest sensitivity to spark advance, as the estimated flame speeds are highest for Case 1.

Due to the nature of the fuel delivery system and valve strategy used in this engine study, it is likely that compositional stratification played a role in the combustion behavior, especially at the earliest spark timings. Thus, global parameters may not be the most relevant metrics to use for comparison with the observed trends. As a consequence, estimates for local conditions were also considered. The previously discussed KIVA-3V model of the engine was used to determine the pressure, temperature, composition, and turbulence characteristics for each Case within a 1 cm^3 volume surrounding the spark plug at the time of spark. The cylinder pressures predicted by KIVA-3V for each Case at the time of spark typically differed from the experimentally measured values by no more than 1-2%.

The estimated local unburned gas temperatures near the spark plug are presented in Figure 8a. The local T_u follows a similar trend to the global results shown in Fig. 7a, with the EGR dilute Case 3 exhibiting the highest T_u for a given spark timing. The magnitudes of the local T_u are elevated by ~3-10% (~30-60 K) compared to the global estimates presented in Fig. 7a since they were determined in the core of the combustion chamber. The results for the local fuel-to-air equivalence ratio (ϕ) and fuel-to-charge equivalence ratio (ϕ') are presented in Figures 8b and 8c, respectively. The increase in ϕ and ϕ' with spark advance indicates an increased concentration of fuel near the spark plug at earlier crank angles, likely due to insufficient mixing of the injected fuel and air/EGR charge. Case 3 consistently has the highest ϕ since it has the highest EGR fraction, but both ϕ and ϕ' at the time of spark increase in a similar manner for all three Cases with spark advance. While fuel stratification appears to be the dominant effect, the KIVA results suggest that insufficient mixing of the residual gases retained during NVO and the incoming air/EGR charge could also be contributing to the behavior. The details of the mixing process are complex and beyond the scope of the current work.

The T_b and S_L determined from the local state using the correlation in [13] are shown in Figures 9a and 9b, respectively, and demonstrate substantially different behavior compared to the global analysis

presented in Fig. 7. Despite the decrease in the local T_u with spark advance, T_b increases for all of the Cases due to the increased ϕ' of the local mixture, provided that the local ϕ is not rich. This is apparent for Case 3 at a spark timing of 60° bTDC, where although Case 3 has the highest T_u and similar ϕ' to the other Cases, it exhibits the lowest T_b due to a lack of air near the spark plug, preventing the complete release of the local charge's chemical energy. For spark timings at or later than 50° bTDC, where all of the mixtures are stoichiometric or lean at the spark plug, the T_b 's are similar for similar T_u and ϕ' , as expected. The estimated local S_L 's in Fig. 9b show a similar behavior to the local T_b . The highest estimated values for S_L are for the Case 1 conditions, which also showed the greatest sensitivity to spark advance experimentally. The Case 2 conditions show a decrease in S_L around the same spark timing that the spark ceased having a noticeable effect on combustion behavior. The most EGR dilute Case 3 conditions, which showed no reaction to the spark event, exhibit the lowest predicted S_L for a given spark timing.

3.3 Assessing flame limit behaviors

As mentioned previously, two conditions limiting the effectiveness of the flame are expected within the current study, namely quenching and limited time for the flame to noticeably affect the overall combustion process. Regarding the latter limiting condition, Figure 10a presents the ratio of ignition delay time (τ_{ID}) to flame time (τ_F) at the time of spark for each condition. The ignition delay time (τ_{ID}) was calculated using the mean cylinder conditions at the time of spark and the iso-octane ignition delay correlation of He et al. [47]. It provides a qualitative estimate for the amount of time it would take the global mixture to auto-ignite at these conditions, neglecting the effects of piston and/or flame front compression, which will tend to reduce the ignition delay. Neglecting these effects, τ_{ID} represents a conservative upper bound when calculated at the time of spark.

The flame time (τ_F), which represents the time it takes for the flame to travel the characteristic distance equal to its thickness, was estimated using $\tau_F = \delta/S_L$ where the laminar flame speed (S_L) and the laminar flame thickness (δ) were determined using the local state conditions near the spark plug at the

time of spark and the correlations of Middleton et al. [13]. The ratio τ_{ID}/τ_F gives an estimate for the number of flame thicknesses traveled during the ignition delay period, and the fraction of flame-based heat release would be expected to increase with increasing τ_{ID}/τ_F for SACI combustion in the absence of factors such as stratification or flame quenching. The results in Fig. 10a suggest that at more retarded spark timings the ignition delay time becomes relatively short compared to the flame time. Trend-wise, this result is expected given that combustion is starting closer to top dead center. The ratio is smallest for the Case 3 condition at a spark advance of 30° bTDC, where no substantial response to spark assist was seen experimentally.

To determine a value for τ_{ID}/τ_F that corresponds to a detectably large fraction of flame-based heat release (i.e. greater than 10%), a SACI dataset presented in Olesky et al. [43] was utilized. This dataset was collected on the same engine under similar operating conditions, where the fraction of flame-based heat release was manipulated via changes to the unburned charge temperature and spark timing at constant combustion phasing. Figure 10b shows the estimated τ_{ID}/τ_F for the dataset from Olesky et al. [43] plotted against the mean estimated fraction of flame-based heat release. The trend line is extrapolated down to “flame-based” heat release levels characteristic of HCCI combustion, i.e. a maximum of 10%. The corresponding τ_{ID}/τ_F is ~50, indicating that even if flames were present under these conditions, they are not likely to be detected with heat release analysis due to the uncertainty in distinguishing between flames and intermediate temperature heat release of the end-gas.

In Fig. 10a, the estimated τ_{ID}/τ_F ratios approach the $\tau_{ID}/\tau_F = 50$ limit at the latest spark timing of 30° bTDC, but are still greater than this value (note that the scale of the y-axis is logarithmic). While approximate, this result suggests that all of the conditions likely have τ_{ID}/τ_F values that are sufficiently high to produce a noticeable increase in the average fraction of flame-based heat release and advance combustion compared to the HCCI conditions, provided that flames can exist. For the conditions where $\tau_{ID}/\tau_F > 50$ and the mean combustion behavior shows little variation compared to the HCCI conditions (e.g. all of the Case 3 conditions), it is reasonable to infer that flame quenching has occurred, at least for a majority of the cycles, given the relatively long ignition delay times available for flame propagation.

3.4 Comparing data to theoretical combustion regimes

Having established flame quenching as the likely cause of combustion non-response and flame limiting behavior for this dataset, the estimated global and local state conditions were plotted on the Leeds diagram [20] in Figure 11 to compare the data to the theoretical regimes of turbulent combustion. The Leeds diagram represents the influence of turbulence on the likelihood of flame quench by flame-turbulence interactions. The flame characteristics (S_L and δ) determined from the correlation in Middleton et al. [13] based on the estimates for the global state conditions in the cylinder are shown in Figure 11a, while the estimates based on the local flame data determined using the KIVA-3V results in the vicinity of the spark plug are plotted in Figure 11b. Additionally, the KIVA-3V engine model was used to estimate the root mean square (rms) turbulent velocity (u') and integral length scale (L) within the 1 cm³ volume around the spark plug at the time of spark. Since the turbulence characteristics near the spark plug are insensitive to changes in mixture composition, the estimated values for u' and L were used for both the global state analysis (Fig. 11a) and the local state analysis (Fig. 11b). Within the range of experimental spark timings, the values of u' and L ranged from 370-450 cm/s and 0.39-0.65 cm, respectively. The theoretical flame quench limits of Abdel-Gayed et al. [20, 48] and Roberts et al. [17] are also included in Figs. 11a and 11b as a function of the Karlovitz number (Ka) as defined by Abdel-Gayed et al. [20, 48] in Eq. 2.

$$Ka = 0.157 \left(\frac{u'}{S_L} \right)^{3/2} \left(\frac{L}{\delta} \right)^{-1/2} \quad (2)$$

Also included in both figures are the SACI data shown in Fig. 10b from Olesky et al. [43] where viable flames were experimentally observed on a cyclic basis, as well as some stable stoichiometric throttled SI data that were collected on the same engine. The flame characteristics for these SACI and SI points were modeled in KIVA-3V by Middleton [35].

Due to high cyclic variability, it was decided that the conditions in Fig. 2 in which the mean CA50 fell outside $\pm 2\sigma$ of the corresponding HCCI CA50 distribution were clearly affected by the spark

event, and therefore, labeled as unquenched. In Figures 11a and 11b, these conditions are indicated by open symbols. The conditions that were defined as quenched have a mean CA50 inside $\pm 2\sigma$ of the HCCI CA50 spread and are shown with closed symbols in both figures. The majority of the quenched data points lie in the appropriate flammability region of the Leeds diagram [17, 20], but the local conditions in Fig. 11b have better agreement with the theoretical regimes of turbulent flame propagation than the global conditions in Fig. 11a. For many of the air dilute Case 1 conditions, the Karlovitz numbers determined from the global state are 20-40 times higher than the Ka calculated from the local state. The findings indicate the shortcomings of the global state analysis and the importance of compositional stratification to the effectiveness of spark assist under the observed experimental SACI conditions. From a practical standpoint, the results suggest that in-cylinder stratification, achieved through various mixing and/or fuel injection strategies, can be used as an additional means of SACI combustion control.

4. Conclusions

In this study, the ability of flames to affect the combustion phasing of highly dilute mixtures with varying ratios of air to EGR dilution was explored. The conditions presented were selected to fall near the boundary between the HCCI and SACI combustion regimes at approximately 4 bar (0.4 MPa) net indicated mean effective pressure (IMEP_n). Starting with three baseline HCCI conditions at constant chemical energy content and combustion phasing, but with varying fractions of EGR, spark assist was implemented at several timings and the combustion response was observed. The following conclusions were drawn:

1. The sensitivity of combustion phasing to spark advance was in part a function of dilution method. At the highest level of EGR dilution, combustion phasing was not affected by spark assist, while at the lowest level of EGR dilution, combustion phasing was noticeably advanced by spark assist. At a spark advance of 80° before TDC, for example, the combustion phasing of the most air dilute mixture ($\phi = 0.62$) advanced by $\sim 8^\circ$ CA on average compared to the HCCI phasing, while the most EGR dilute mixture ($\phi = 0.97$) showed almost no response to the spark event, despite

the fact that the unburned gas temperature in the vicinity of the spark plug was highest for the EGR dilute mixture. For these conditions, the combustion behavior resembled that of HCCI.

2. For a distribution of cycles at a given spark timing, the most advanced cycles demonstrated a larger fraction of flame-based heat release and earlier end-gas auto-ignition. This observation indicated that the increased levels of dilute flame propagation and associated end-gas compression contributed to the advance in combustion phasing.
3. As the spark was advanced up to 105° before TDC for the most air dilute mixture, combustion stability deteriorated and the spread in CA50 for 200 consecutive cycles increased. Alternatively, for the more EGR dilute mixtures the combustion stability remained approximately constant, regardless of spark timing. The use of spark assist, therefore, does not consistently increase the stability of dilute combustion.
4. In comparing the estimated ignition delay time (τ_{ID}) to the flame time (τ_F) calculated in part with KIVA-3V predictions for each condition, it was found that τ_{ID} increased compared to τ_F as spark advanced. This indicated that, at more advanced spark timings, the absence of deflagrative heat release and combustion advance likely resulted from flame quench rather than a lack of time for the flame to be effective.
5. The results of a detailed KIVA-3V model of the engine indicated that the in-cylinder mixture became increasingly stratified at more advanced crank angles. For a given spark timing and turbulent flow field, the flame characteristics estimated from the local conditions near the spark plug were more consistent with the theoretical regimes of turbulent combustion presented in the Leeds diagram [20] than the flame characteristics estimated from the global cylinder state. This finding indicates that a bulk properties analysis fails to explain the experimental observations, and in-cylinder stratification can highly affect the behavior and effectiveness of SACI within a practical combustion device.

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657

658 **Nomenclature**

659 AKI anti-knock index

660 aTDC after top dead center

661 bTDC before top dead center

662 CA crank angle

663 CA50 combustion phasing; crank angle where 50% of fuel mass is burned

664	CoV	coefficient of variation
665	δ	laminar flame thickness
666	EGR	exhaust gas recirculation
667	HCCI	homogeneous charge compression ignition
668	HR	heat release
669	IMEP _n	net indicated mean effective pressure
670	L	turbulent integral length scale
671	LTC	low temperature combustion
672	Ka	Karlovitz number
673	MBT	maximum brake torque
674	NVO	negative valve overlap
675	ϕ	fuel-to-air equivalence ratio
676	ϕ'	fuel-to-charge equivalence ratio
677	rms	root mean square
678	σ	standard deviation
679	SACI	spark assisted compression ignition
680	SI	spark ignited
681	S_L	laminar flame speed
682	T_b	burned gas temperature
683	TDC	top dead center
684	T_u	unburned gas temperature
685	τ_{ID}	ignition delay time
686	τ_F	flame time
687	u'	rms turbulent velocity
688		
689		

Figure Captions

- 690 **Figure 1:** 3-D computational mesh used in the KIVA-CFMZ model containing 156,000 cells and
691 corresponding to the geometry of the metal engine used in the study.
- 692 **Figure 2:** Response of CA50 to spark advance for the three Cases listed in Table 3. Data at 0° spark
693 timing are for the baseline HCCI conditions where no spark was used. Each dataset contains 200
694 consecutive cycles of pressure data. The diamond-shaped symbols are mean CA50 values. The dashed
695 lines are $\pm 2\sigma$ in CA50 for the HCCI conditions.
- 696 **Figure 3:** Histograms of CA50 containing 200 consecutive cycles for each condition presented in Figure
697 2 – (a) Case 1, (b) Case 2, and (c) Case 3. Spark advance (SA) values are presented in crank angle
698 degrees before TDC.
- 699 **Figure 4:** Heat release profiles of three individual cycles for Case 1 at a spark advance of 90° bTDC.
700 Each curve represents an individual cycle (out of 200): the most advanced cycle (minimum CA50), the
701 most retarded cycle (maximum CA50), and the cycle whose CA50 falls closest to the mean value. Note
702 that the most retarded cycle resembles HCCI combustion.
- 703 **Figure 5:** Estimated fraction of flame-based heat release (HR) as a function of CA50 for each cycle of the
704 Case 1 conditions shown in Figure 3a. The dashed lines represent the range of values determined from
705 the baseline HCCI condition (~4-10%). The cycles with flame-based heat release above this range are
706 advanced due to spark-induced flame propagation.
- 707 **Figure 6:** (a) CoV of IMEP_n and (b) engine-out NO_x emissions as a function of spark advance for each
708 condition shown in Figure 2. Data at 0° spark advance are for the baseline HCCI conditions.
- 709 **Figure 7:** (a) Estimated mean global values of unburned gas temperature (T_u) at the time of spark from
710 heat release analysis; estimated values of (b) burned gas temperature (T_b) and (c) laminar flame speed (S_L)
711 determined from the mean global state at the time of spark using the correlation of Middleton et al. [13].
- 712 **Figure 8:** Estimated local values of (a) unburned gas temperature (T_u), (b) fuel-to-air equivalence ratio
713 (ϕ), and (c) fuel-to-charge equivalence ratio (ϕ') at the time of spark determined from the KIVA-3V
714 engine model [34] within a 1 cm³ volume around the spark plug.
- 715 **Figure 9:** Estimated values of (a) burned gas temperature (T_b) and (b) laminar flame speed (S_L)
716 determined from the local state at the time of spark using the laminar flame speed correlation of
717 Middleton et al. [13].
- 718 **Figure 10:** (a) Ratio of ignition delay time (τ_{ID}) to flame time (τ_F) calculated at the time of spark for each
719 condition. Note that the y-axis is a logarithmic scale. (b) τ_{ID}/τ_F plotted against the mean fraction of flame-
720 based heat release for SACI data presented in Olesky et al. [43]. Extrapolating the trend line to flame-
721 based heat release fractions of 10% yields a value for τ_{ID}/τ_F of ~50, which is the value where heat release
722 due to the flame is projected to be indistinguishable from the intermediate temperature heat release of the
723 end-gas.
- 724 **Figure 11:** Leeds diagram showing estimates of the flame characteristics using (a) the global state at the
725 time of spark and (b) the local state in the vicinity of the spark plug determined from KIVA-3V [34] at the
726 time of spark. Flame quenching was defined to occur for the conditions in which the mean CA50 was

727 within $\pm 2\sigma$ of the CA50 distribution for the baseline HCCI Cases. These conditions are represented by
728 closed markers and non-quenching conditions are represented by open markers.

729

Table 1: Engine geometry

Parameter	Value
Displaced volume (cm ³)	550
Bore (mm)	86.0
Stroke (mm)	94.6
Connecting rod length (mm)	156.5
Piston pin offset (mm)	0.8
Compression ratio	12.5:1

Table 2: Settings of fixed engine parameters

<i>Parameter</i>	<i>Value</i>
Engine speed (rpm)	2000
Fuel flow rate (mg/cycle)	12.5
Fuel injection pressure (bar)	100
Start of fuel injection (° bTDC)	330
End of fuel injection (° bTDC)	309
Negative valve overlap (° CA)	152
Intake valve closing (° bTDC)	150
Exhaust valve opening (° aTDC)	150
Valve lift (mm)	6.0
Engine coolant/oil temperature (° C)	90
EGR coolant temperature (° C)	55
Spark energy from the coil (mJ)	70

Table 3: Unburned mixture properties of the baseline HCCI Cases with varying levels of air to EGR dilution

<i>Parameter</i>	<i>Case 1</i>	<i>Case 2</i>	<i>Case 3</i>
Fuel-to-air equivalence ratio, ϕ	0.62	0.81	0.97
Fuel-to-charge equivalence ratio, ϕ'^a	0.37	0.38	0.38
External EGR volumetric fraction, measured in intake manifold (%)	0	21	31
External EGR mass fraction, in-cylinder (%) ^a	0	12	17
Internal EGR (residual) mass fraction (%) ^a	40	41	43
Total EGR mass fraction (%) ^a	40	53	60
Molar O ₂ fraction in unburned mixture (%) ^a	15.6	12.1	9.3
Intake charge temperature (° C)	45	77	115
Intake pressure (bar, absolute)	1.0	1.04	1.08
Exhaust pressure (bar, absolute)	1.05	1.08	1.12
Ringling intensity (MW/m ²)	3.1	2.4	1.9
CoV of IMEP _n (%)	0.98	1.36	1.53

^a Derived quantities based on inferred internal EGR (residual) mass from heat release analysis

Figure 1: 3-D computational mesh used in the KIVA-CFMZ model containing 156,000 cells and corresponding to the geometry of the metal engine used in the study.

Figure 2: Response of CA50 to spark advance for the three Cases listed in Table 3. Data at 0° spark timing are for the baseline HCCI conditions where no spark was used. Each dataset contains 200 consecutive cycles of pressure data. The diamond-shaped symbols are mean CA50 values. The dashed lines are $\pm 2\sigma$ in CA50 for the HCCI conditions.

(a) Case 1

(b) Case 2

(c) Case 3

Figure 3: Histograms of CA50 containing 200 consecutive cycles for each condition presented in Figure 2 – (a) Case 1, (b) Case 2, and (c) Case 3. Spark advance (SA) values are presented in crank angle degrees before TDC.

Figure 4: Heat release profiles of three individual cycles for Case 1 at a spark advance of 90° bTDC. Each curve represents an individual cycle (out of 200): the most advanced cycle (minimum CA50), the most retarded cycle (maximum CA50), and the cycle whose CA50 falls closest to the mean value. Note that the most retarded cycle resembles HCCI combustion.

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Figure 8: Estimated local values of (a) unburned gas temperature (T_u), (b) fuel-to-air equivalence ratio (ϕ), and (c) fuel-to-charge equivalence ratio (ϕ') at the time of spark determined from the KIVA-3V engine model [34] within a 1 cm^3 volume around the spark plug.

Figure 9: Estimated values of (a) burned gas temperature (T_b) and (b) laminar flame speed (S_L) determined from the local state at the time of spark using the laminar flame speed correlation of Middleton et al. [13].

Figure 10: (a) Ratio of ignition delay time (τ_{ID}) to flame time (τ_F) calculated at the time of spark for each condition. Note that the y-axis is a logarithmic scale. (b) τ_{ID}/τ_F plotted against the mean fraction of flame-based heat release for SACI data presented in Olesky et al. [43]. Extrapolating the trend line to flame-based heat release fractions of 10% yields a value for τ_{ID}/τ_F of ~ 50 , which is the value where heat release due to the flame is projected to be indistinguishable from the intermediate temperature heat release of the end-gas.

Figure 11: Leeds diagram showing estimates of the flame characteristics using (a) the global state at the time of spark and (b) the local state in the vicinity of the spark plug determined from KIVA-3V [34] at the time of spark. Flame quenching was defined to occur for the conditions in which the mean CA50 was within $\pm 2\sigma$ of the CA50 distribution for the baseline HCCI Cases. These conditions are represented by closed markers and non-quenching conditions are represented by open markers.