



On the Phenomenology of Hot-Spot Induced Pre-Ignition in a Direct-Injection Hydrogen-Fueled, Heavy-Duty, Optical-Engine

Rajavasanth Rajasegar and Ales Srna Sandia National Laboratories, Livermore, CA, United States

Ibrahim Barbery and Ricardo Novella CMT – Motores Térmicos, Universitat Politècnica de València, Camino de Vera, 46022 Valencia, Spain

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Abstract

Hydrogen-fueled internal combustion engines are highly susceptible to pre-ignition from external sources due to its low minimum ignition energy despite the hydrogen's good auto-ignition resistance. Pre-ignition leads to uncontrolled abnormal combustion events resulting in knocking and / or backfire (flashback) which may result in mechanical damage, and as such represents tenacious obstacle to the development of hydrogen engines. Current pre-ignition mitigation strategies force sub-optimal operation thereby eroding the efficiency / emissions advantages of hydrogen fuel making the technology less attractive. Hydrogen pre-ignition phenomenon is poorly understood and knowledge gaps about the underlying mechanisms remain.

To this end, a phenomenological study of hot-spot induced pre-ignition is carried out in a direct-injection hydrogen-fueled, heavy-duty, single-cylinder optical engine. Pre-ignition is induced with an electrically heated glow-plug which creates

a hot-spot with varying surface temperatures based on the applied excitation voltage. The effect of engine speed, hot-spot temperature and hydrogen injection timing on pre-ignition frequency and phasing is studied using optical diagnostics. First, the hot-spot temperature during engine operation is characterized using infrared (IR) imaging, which relied on pre-calibration using thin wire thermocouple. Thereafter, the mixture field surrounding the glow-plug is characterized by tracer PLIF using hydrogen seeded with anisole. High-speed OH* chemiluminescence imaging is used in conjunction with cylinder pressure measurements to characterize pre-ignition timing. Experimental results are complemented with closed homogeneous reactor chemical kinetic calculations to understand the effect of varying in-cylinder temperature and pressure on hydrogen ignition delay. An interplay between surface temperature, in-cylinder pressure, and injection timing is revealed, which explains the tendency of pre-ignition to occur during the gas-exchange or in early compression stroke.

Introduction

A promising solution for de-carbonization of transportation, combined heat and power systems (CHP), and power generation is to integrate the use of carbon-neutral fuels [1]. Among these technologies, hydrogen-fueled Internal Combustion Engines (ICE's) gained attention of both OEMs and regulators due to their durability, robustness, lower manufacturing costs and reduced noble metal usage when compared to Fuel-Cell Electric Vehicles (FCEV's) [2, 3, 4, 5, 6]. As a fuel, hydrogen (H₂) has several properties that make it attractive for combustion applications, such as wide flammability limits, high flame speed [7, 8], good auto-ignition resistance [9], and the fact that it can be produced using renewable energy sources [10].

Many research efforts during the past years have focused on mid-term solutions for commercial light-duty and heavy-duty engines by retrofitting existing engines and substituting part of conventional fuel with hydrogen [11, 12, 13, 14]. Gasoline-fueled spark-ignition (SI) engine combined with small amounts of hydrogen injected in the intake port have shown great potential to operate at very lean conditions ($\lambda \sim 1.9$) with high efficiency and low Nitrogen Oxides (NOX) emissions [15]. Hydrogen addition has shown potential for lean-limit extension and reduced NOX emission in light-duty natural gas (NG) fueled SI engines [16]. Additional light-duty works focused on hydrogen benefits on cycle-to-cycle variability (CCV) [17, 18], NOX formation [19], lean-limit extension [20], performance and emissions [21]. This approach is

also attractive for larger engines [22] considering the wide-spread adoption of natural gas in heavy-duty transportation.

Engines operating on 100% H₂ can further reduce the tailpipe CO₂ emissions towards near-zero value. However, several barriers in development of H₂ ICE associated with power density, fuel injection technology, and mitigation of pre-ignition need to be resolved before H₂ ICE can directly substitute the existing diesel and natural-gas powertrains [3, 23, 24]. In particular, pre-ignition and related back-fire are important constraints that limit engine power-density, transient response, and efficiency [3, 23, 24, 25]. Here, pre-ignition is defined as spontaneous initiation of combustion ahead of the desired ignition timing, and results in high in-cylinder pressure and/or combustion knock [26, 27]. If pre-ignition occurs during the intake stroke, flame will propagate into the intake port and may compromise its mechanical integrity – this is a particularly high risk for port-injected engine designs.

The high auto-ignition resistance of H₂ under engine conditions can help to avoid knock, however, the low H₂ minimum ignition energy makes H₂ especially prone to pre-ignition [28, 29]. Despite the wealth of knowledge on low-speed pre-ignition in gasoline direct-injection (GDI) engines, hydrogen fuel does not wet cylinder walls, which is the root-cause of pre-ignition in GDI engines [30]. Though turbulence mixing with colder boundary layers has shown to increase ignition delay times, pre-ignition especially at lower pressures and increased ignition delay times have been attributed to the thermal diffusivity of the mixture [31], which becomes significant in the case of hydrogen. Several potential mechanisms of pre-ignition identified in the literature include hot-spots in combustion chamber (exhaust valves, spark plug) [32, 33, 34], catalytic effects on platinum spark-electrodes [35], hot residuals from previous cycle [36], auto-igniting oil-droplets, hot particles, hot (carbonaceous) deposits on engine walls [37] and slowly-burning flame in the top-land crevice [38]. The plethora of potential sources of pre-ignition, lack of the fundamental understanding behind each individual mechanism, and a wide range of engine designs in the market makes efficient mitigation of pre-ignition challenging. With the lack of understanding and systematic studies of pre-ignition under controlled conditions, it is often unclear which pre-ignition mechanism is dominant. In port-injected engines, optimization of valve and injection timing can often reduce the back-fire tendency by reducing the interaction of fresh charge with hot exhaust residuals [25, 32]. At higher loads and with direct-injection technologies, other pre-ignition mechanisms become dominant, and the best mitigation approaches are less clear.

Therefore, the objective of this study is to enhance the understanding of one potential pre-ignition mechanism in a Direct Injection (DI) SI hydrogen engine – hot-spot induced pre-ignition. For this purpose, an artificial hot-spot with adjustable surface temperature was introduced into the engine combustion chamber to observe how the hot-spot temperature and injection timing impact the frequency and the timing of pre-ignition. High-speed OH* chemiluminescence imaging was used to detect the timing of pre-ignition. Several injection timings were tested at two engine operating speeds, and for each test, multiple surface temperatures of the hot-spot were evaluated. Finally, the experimental results are complemented with 0-D chemical kinetics well-stirred reactor calculations

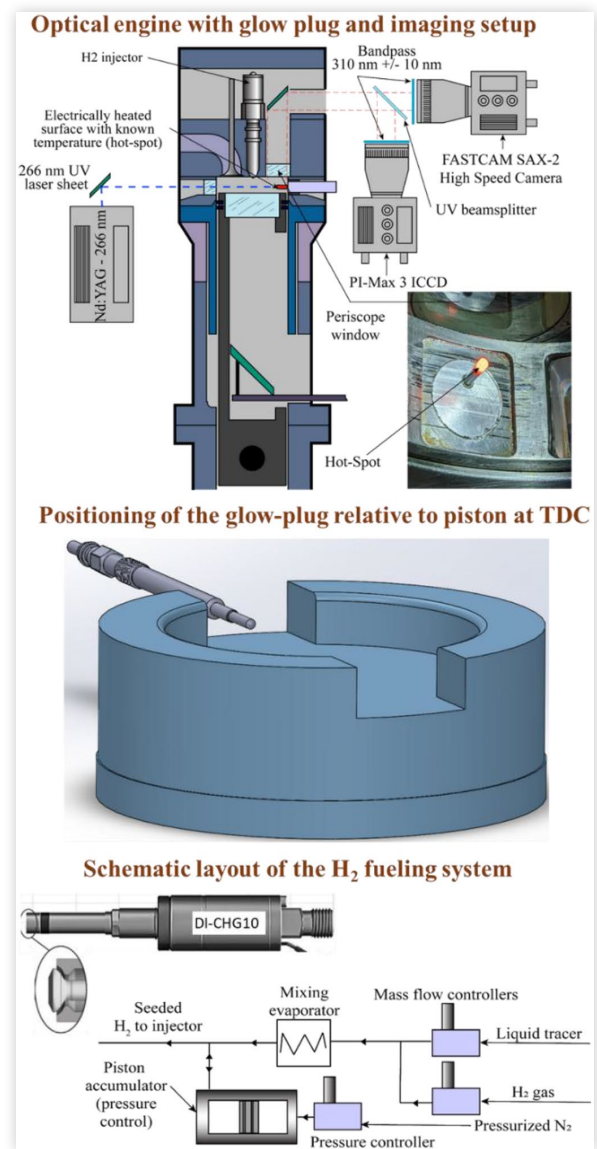
to gain fundamental insights on mechanisms behind the hot-spot induced pre-ignition in hydrogen ICE.

Experimental Overview

Optical Engine, Fuel System, and Artificial Hot-Spot

The experiments were conducted in the Sandia Heavy-Duty Optical Engine, which is modified from a single-cylinder Cummins N-14 series direct-injection heavy-duty diesel engine with a displacement of 2.34 L and compression ratio of 10.3:1 in the configuration used here. A cross-section schematic of the experimental arrangement is shown in Figure 1, with the main

FIGURE 1 Schematic of the optical engine setup (top) and layout of the gaseous fuel supply system with tracer seeding setup (bottom).



experiment properties summarized in Table 1. The engine piston features a 15.5 mm deep cylindrical non-re-entrant bowl with 97.8 mm diameter. The bowl-rim is interrupted with two 37 mm wide and 15.5 mm deep cutouts spaced 180° apart to enable optical diagnostics and to avoid the piston shearing the glow-plug (hot-spot) protruding into the combustion chamber, as further discussed below. The engine working fluid can be air, air diluted with nitrogen, or neat nitrogen, and the intake temperature is conditioned with an electrical heater. The cylinder pressure is measured with an AVL QC43D piezoelectric pressure transducer and recorded every 0.25 crank-angle degree (CAD). A detailed description of this engine can be found in the literature [39, 40, 41].

The engine was fueled with hydrogen using a central-mounted direct-injection, medium-pressure outward-opening injector (BorgWarner, DI-CHG10) with a maximum flow rate of 10 g/s. The far-field flow-pattern of this injector resembles a single-hole nozzle flow – the initial hollow-cone jet rapidly collapses and the momentum of the resulting flow is primarily aligned with the injector axis, with limited axial spreading [42].

For experiments measuring the local equivalence ratio near the glow-plug, pressurized H₂ gas was seeded with 0.1 volume-% of vaporized tracer blend consisting of 8% anisole and 92% iso-octane. Due to the low molecular weight of hydrogen, it is a challenge to effectively track hydrogen using a tracer due to the differences in the transport properties [42]. However, for the purposes of this study, it is reasonable to

assume that the spatial distribution of the tracer is representative of in-cylinder hydrogen concentration. The tracer blend and H₂ streams with precisely controlled flowrates were mixed at a reduced pressure of 5 bar by a Bronkhorst Controlled Evaporator-Mixer system (CEM, model W-303A). This tracer-seeded H₂ stream filled a piston accumulator with 6 L displacement. Once full, the seeded H₂ gas was compressed by pressurized nitrogen in the other cavity of the piston accumulator. A piston with Kalrez seals prevented the two gases from mixing. The nitrogen pressure was controlled by a pressure controller (Tescom ER5000 actuating a dome-loaded regulator) to ensure repeatable injection pressure. Each batch of seeded H₂ was sufficient for about 80 fuel injections. Diluting the anisole with iso-octane was necessary to avoid condensation of anisole in the piston accumulator.

A glow-plug (Bosch DuraSpeed) was used as a hot-spot with adjustable temperature. A custom-designed holder positioned the glow-plug in horizontal orientation, with the glow-plug axis about 16 mm below the fire-deck. The cylindrical glow-plug tip with 3 mm diameter protruded to 13 mm radial distance from the cylinder wall. A bowl-rim design with 37 mm wide and 15.5 mm deep cutout aligned with the glow-plug location prevented the piston from shearing the glow-plug tip when approaching the top-dead center (TDC). The glow-plug temperature was open controlled by modifying the applied excitation voltage without any feedback. The glow-plug temperature is highest at its tip with a maximal nominal temperature of 1570 K.

TABLE 1 Engine, fuel injector and glow plug specifications.

Engine Specifications	
Engine base type	Cummins N-14, DI diesel
Number of cylinders	1
Number of intake valves	2
Number of exhaust valves	1*
Combustion Chamber	Quiescent, direct injection
Swirl ratio	0.5
Bore x Stroke [mm]	139.7 x 152.4
Compression ratio [-]	10.3:1
Bowl Width-Depth [mm]	97.8
Bowl Depth [mm]	15.5
Displacement [liters]	2.34
Connecting rod length [mm]	304.8
Fuel injector	
Hydrogen injector	BorgWarner, DI-
Flow Rate	Up to 10 g/s of H ₂
Mounting location	Centrally mounted in the cylinder head
Glow plug characteristics	
Glow-plug type	Bosch Duraspeed
Hot-spot tip location	16 mm below fire deck, 13 mm radially inwards from cylinder wall
Maximum temperature	1570 K (nominal) 1210 K (tested during engine operation)

* In this optically accessible diesel engine, one of the two exhaust valves of the production cylinder head is replaced by a window.

Optical Diagnostics

Optical diagnostics in this study used optical access through a 50 mm diameter fused-silica window replacing one of the two exhaust valves and another window in the cylinder liner positioned diametrically opposite of the hot-spot. The window in the Bowditch-piston was not used. A bowl-rim design with two 37 mm wide and 15.5 mm deep cutouts was used to prevent the bowl-rim from blocking the cylinder-liner window when piston is near TDC (see Figure 1).

OH* chemiluminescence imaging was used to characterize pre-ignition timing at different hot-spot temperatures and hydrogen injection timings. For this purpose, a high-speed CMOS camera (Photron FastCam SA-X2) coupled to a high-speed UV intensifier (Lambert Instruments HiCATT, S20 photocathode) equipped with a Cerco 100mm f/2.8 UV lens and a 310±5nm bandpass filter (Edmunds Optics #34-980) was employed. The camera was operated at 10 kHz frame rate, intensifier gate of 90 µs, 640x640 pixel resolution and projected pixel size of 0.08 mm/pixel. The pre-ignition timing was assumed to correspond to the first detected OH* emission.

Tracer-PLIF was used to study the mixture formation near the glow-plug. A 4th harmonic of a 10 Hz Nd:YAG laser (Spectra-Physics GCR-270) with pulse energy of 12 mJ/pulse and a wavelength of 266 nm was used phase-locked with engine rotation. The 35 mm wide and roughly 1 mm thick laser light-sheet entered the engine through the window in the cylinder liner. A +1000 mm focal length spherical lens and

a cylindrical micro-lens array with a nominal divergence angle of 2.3° were used as light-sheet forming optics.

A UV-sensitive ICCD camera (Princeton Instruments PI-MAX3, SB photocathode), equipped with a Cerco 45 mm f/1.8 UV lens and a 310 ± 15 nm band-pass filter (BPF) (Edmunds #12-097 and Schott GG295) was used to detect the emitted tracer fluorescence signal while the glow-plug was disabled to avoid temperature stratification. The projected pixel size was roughly 0.09 mm/pixel. The camera was synchronized to the laser and operated at an intensifier gate of 500 ns.

Glow Plug Characterization

Infrared (IR) imaging was used to characterize the glow-plug temperature dependence on supply voltage during the engine operation. A Telops TS-IS InSb IR camera imaging the mid-infrared emission from the hot-spot was used to estimate the hot-spot temperature. The camera view was directed through the exhaust valve window in the cylinder head. First, the camera was calibrated by wrapping a 0.003" thin-wire K-type thermocouple around the glow-plug to measure its surface temperature and correlating the detected IR emission brightness to temperature using procedure described in [43]. The uncertainty in temperature estimation based on the calibration of the IR intensity is conservatively estimated to be less than 10 K. Next, the calibrated camera was used to record the IR emission from the glow-plug at varying supply voltage during the engine operation to characterize the surface temperature dependence on supply voltage (Figure 2). This was found crucial to characterize the glow-plug temperature during engine operation because of the strong convective cooling which significantly reduced the glow-plug surface temperature compared to the engine at still-stand.

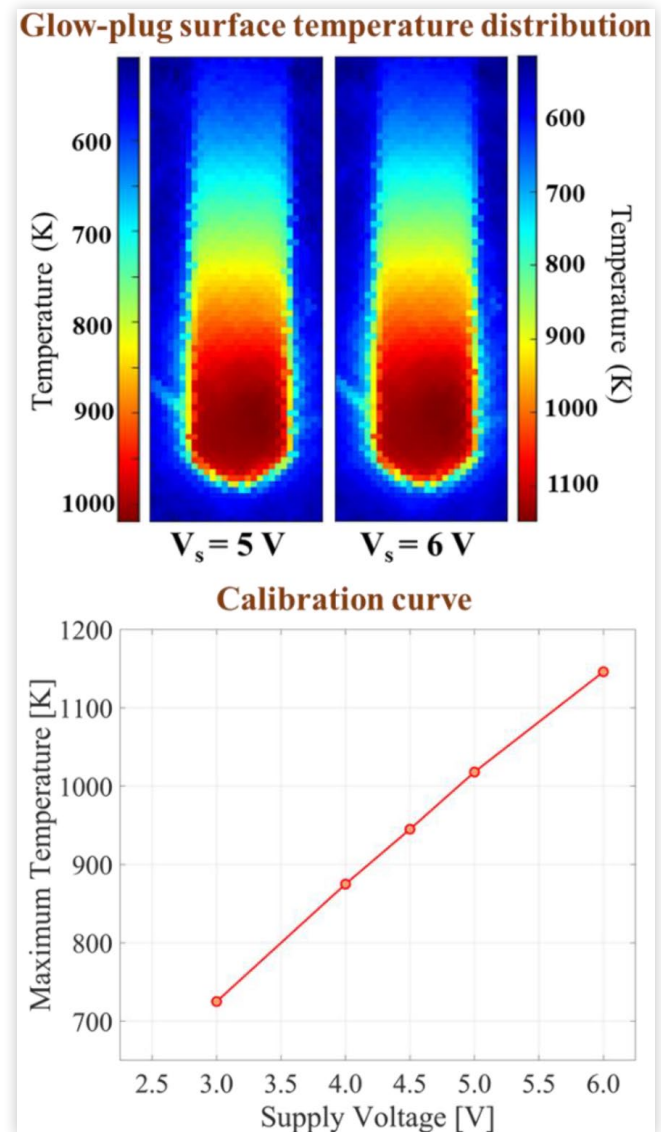
Figure 2 shows the sensitivity of cycle-averaged maximal surface temperature to supply voltage at 1200 RPM (bottom) and the temperature distribution at the glow-plug surface at 5.0 V and 6.0 V supply (top). When operating at supply voltages in-between points with IR characterized temperature, a linear interpolation was used to estimate the hot-spot temperature. As visible from the temperature distribution, the hot area on the glow-plug is limited to roughly 4–5 mm distance from the tip, after which it rapidly decreases. Therefore, pre-ignition is expected to occur in the direct vicinity of the glow-plug tip.

The question of surface temperature changes within the cycle was addressed by acquiring IR images every 30°CA at an engine speed of 1200 RPM. It was confirmed that the thermal inertia of the glow plug is sufficient to prevent fluctuations of the surface temperature within the cycle, which remained constant within the measurement precision of roughly ± 5 K.

Experimental Procedure and Test Matrix

The engine operating conditions are shown in Table 2. The intake pressure (0.95 bar), intake temperature (305 K) and the injected fuel mass (global $\lambda = 3$) were kept constant for the

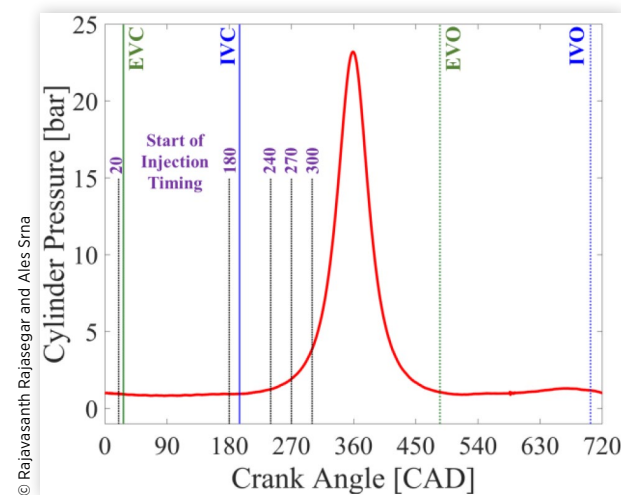
FIGURE 2 IR imaging showing the spatial distribution of temperature along the glow-plug surface at two supply voltages (top). Calibration curve showing the correlation between the maximum hot-spot surface temperature and the applied supply voltage (bottom).



entire measurement matrix. The low intake temperature allowed to minimize any unintended pre-ignition caused by rogue oil droplets originating from the piston rings that were minimally lubricated to reduce friction. The fuel was supplied directly into the cylinder during the intake stroke (SOI = 20 CAD) or compression stroke (SOI is varied from 180 CAD to 300 CAD), with injection pressure of 20 bar and 4.4 ms solenoid energizing time. Figure 3 shows the various injection timing used in this study relative to the valve timing of the optical engine and the in-cylinder back pressure during the hydrogen injection. Ahead of each experimental run, the injection timing and the glow-plug supply voltage (and therefore, the glow-plug temperature) were set. The engine was skip-injected (1 cycle in 10) while the intake/exhaust valves were operated in all cycles to allow for continuous gas

TABLE 2 Engine operating conditions and test matrix.

Experimental Conditions	
Intake temperature [K]	305
Intake pressure [bar]	0.95
Coolant temperature [K]	353
Engine speed [RPM]	600, 1200
Global λ	3
Injection pressure [bar]	20
Injection duration [ms]	4.40
Test matrix	
Injection timing [CAD]	20 180 240 270 300
Glow-plug temperature [K]	1102 1138 1138 1138 1198
	1114 1150 1150 1150 1210
	1126 1162 1162 1162 1222
	1174 1174 1174 1198

FIGURE 3 Motored pressure trace indicating the valve timing and the crank angle convention used in the study along with the hydrogen injection timing.

exchange. In each run, 50 cycles with fuel injection were acquired, while a high-speed camera acquired the OH* signal to determine the pre-ignition timing if it occurred. The “9:1 skip-fired” operation of the optical engine allowed for sufficient time between the fired cycles for the glow-plug to cool-down following heating from the hot combustion gases during pre-ignited cycles. The continuous gas-exchange also eliminated the impact of combustion residual gases due to incomplete scavenging on pre-ignition in the subsequent cycles. Two engine speeds (600 and 1200 RPM) were tested. At each injection timing and engine speed, a span of glow plug temperatures was tested in 12 K increments (0.1 V supply voltage increase) to cover conditions with no pre-ignition until nearly all cycles pre-ignited (> 70%). Since the periscope window provided complete optical access to the glow-plug and the surrounding region, OH* chemiluminescence imaging was used for screening and eliminating any rogue pre-ignition

(less than 15 cycles across the entire data set spanning different injection timings and glow-plug temperatures) that did not originate from the hot-spot for further analysis.

Results and Discussion

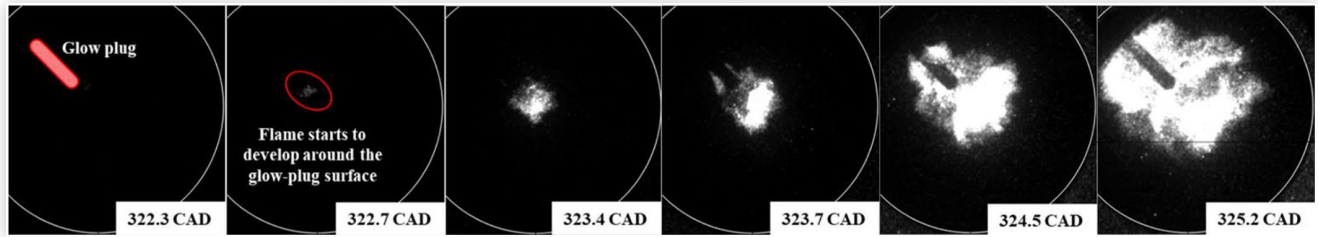
Spatio-Temporal Evolution of Hot-Spot Induced Pre-Ignition

The spatio-temporal evolution of the flame kernel due to the hot-spot induced pre-ignition was characterized using high-speed OH* chemiluminescence imaging. A sequence of selected snapshots showing the typical evolution of the resulting flame kernel due to hot-spot induced pre-ignition at 600 RPM for an SOI = 300 CAD is presented in Figure 4. From the sequence of images, it can be clearly seen that the initial ignition reactions tend to occur on the surface or in a thin boundary layer close to the surface of the glow-plug typically near its tip, where surface temperatures tend to be the highest. The initiated flame kernel leads to flame propagation which first tends to develop along the surface of the glow plug due to the relatively high temperatures near the vicinity of the glow plug. Following this, the flame then propagates away from the glow plug due to convection or favorable mixing that eventually leads to rapid combustion that consumes the fuel-air charge in the rest of the combustion chamber. Though the initial ignition reactions appear to happen on the surface or in close proximity (boundary layer region) to the glow plug, the exact mechanism of these chemical reactions is still unclear. The porosity of ceramic materials used in the glow-plug can potentially harbor active sites that can result in surface chemistry reactions resembling “catalysis”. This is certainly of interest as current spark-plug components contain precious metals like platinum and iridium, which are known catalysts for reactions involving H₂ that can potentially affect pre-ignition tendencies. We plan to pursue this further in the future by probing the catalytic activity of precious metals by coating the glow plug surface with platinum and iridium to study its impact on H₂ pre-ignition tendencies further supplemented by CFD studies including surface-chemistry simulations.

Stochastic Nature of Pre-Ignition Timing

For the operational test matrix presented in Table 2, the pre-ignition phenomenon was characterized in terms of its frequency and its onset timing based on the high-speed OH* chemiluminescence imaging data which was then cross-correlated with thermodynamic cylinder pressure analysis. The first “detectable” occurrence of OH* signal from the high-speed imaging data is considered as the onset of pre-ignition, which was typically about ~5–8 CAD earlier when compared to the estimate based on discernible cylinder pressure rise. The calculated pre-ignition frequency and timing is later correlated to the injection frequency and the glow-plug temperature.

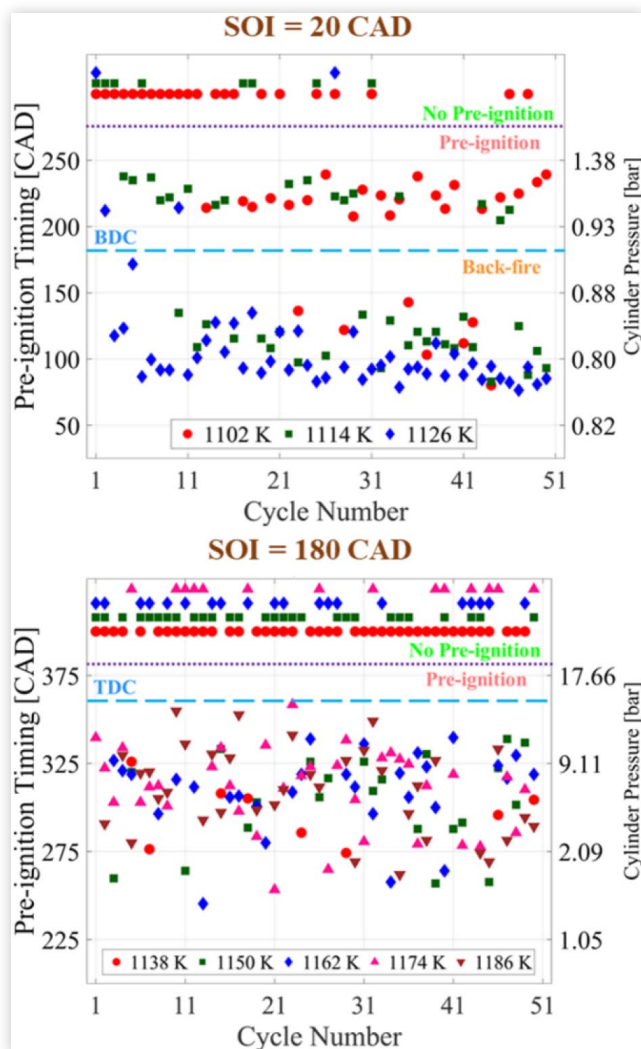
FIGURE 4 Selected representative snapshots of high-speed OH* chemiluminescence images at key timings showing the spatio-temporal evolution of hot-spot induced pre-ignition at 600 RPM and SOI = 240 CAD



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The results of the above analysis are summarized in Figure 5 for early injection timings SOI = 20 CAD and 180 CAD in the top and bottom panels respectively. Each panel presents the calculated timing of pre-ignition onset for a test run consisting of 50 cycles in total at an engine speed of 1200

FIGURE 5 OH* chemiluminescence based pre-ignition frequency (50 cycles in total) and timing (onset) for early injection timings at 1200 RPM for different hot-spot temperatures. Start of injection is 20 CAD (top) and 180 CAD (bottom). Secondary axis indicates the corresponding cylinder pressure for the indicated CAD timings.



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RPM. Cycles that do not pre-ignite are grouped at the top of each panel and labelled accordingly. The corresponding cylinder pressure for the range of indicated CAD is also shown using the secondary axis for reference. For each injection timing, the temperature of the hot spot was progressively increased (in steps of 0.1 V supply voltage corresponding to about ~12 K) so as to initiate a gradual transition from test runs with almost no cycles undergoing pre-ignition to a majority of cycles (> 70%) pre-igniting. This glow-plug temperature sweep is indicated by different colored markers as shown in Figure 5.

For the earliest injection timing, i.e., SOI = 20 CAD, it can be seen that for a hot-spot temperature of 1102 K, around ~55% of the cycles pre-ignite, with around 15% of these cycles, igniting during the intake stroke (before 150 CAD). This phenomenon commonly referred to as backfire or flashback [25, 38] is characterized by the occurrence of pressure waves travelling towards the intake port as combustion tends to “flashback” towards this region. This issue represents a major hurdle to overcome in the development of hydrogen ICE due to the high flammability of the fuel, which is further exacerbated in port-fuel injection systems due to the presence of combustible mixture in the intake port region [41, 42].

As the glow-plug temperature is further increased to 1114 K, around ~85% of the cycles tend to pre-ignite with nearly half of them resulting in backfire. Finally, at a temperature of 1126 K almost all of the cycles pre-ignited during the intake stroke. This temperature sweep indicates a high sensitivity of the pre-ignition phenomenon to the hot-spot temperature, given that a variation of only 12 K was sufficient to cause pre-ignition in a majority of the engine cycles.

For an SOI of 180 CAD, five glow-plug temperatures were evaluated. It is to be noted that for this SOI condition, the minimum temperature (1138 K) required for inducing the pre-ignition in at least one of the cycles is higher than the maximum temperature (1126 K) evaluated for the previous injection timing of 20 CAD. This suggests that with later injection timings, higher hot-spot temperatures might be required to induce pre-ignition. Further, from the spread, it can be seen that the timing of pre-ignition onset appears to be far more stochastic than the earlier case with a majority of the cycles pre-igniting later (around ~100 CAD after the injection). This can possibly be due to the reduced bulk motion within the cylinder following the closure of intake valves, which then requires piston motion to transport the fuel-air mixture close to the glow-plug to initiate pre-ignition.

At a glow-plug temperature of 1138 K, only around ~15% of the cycles pre-ignite and the fraction of cycles tending to pre-ignite increases sharply with increasing hot-spot temperature as shown in Figure 5. Furthermore, among the cycles that do pre-ignite, a stochastic behavior is observable regardless of the glow-plug temperature, with the large spread in the timing of pre-ignition onset ranging anywhere between early during the compression stroke (~250 CAD) to near TDC. This highlights the importance of in-cylinder bulk flow motion and mixture formation that can strongly affect the onset of pre-ignition but likely exhibit high cyclic variability in the configuration used here as investigated in the next section.

Similar sweeps were performed with later injection timings of 240 CAD, 270 CAD and 300 CAD and the results are summarized in the top, middle and bottom panel of Figure 6 respectively. At an SOI of 240 CAD, as shown in Figure 6, for glow-plug temperatures below 1150 K, hardly 5% of the cycles tend to pre-ignite. As discussed earlier, the sensitivity of pre-ignition to the hot-spot temperature is again evident here: At a glow-plug temperature of 1162 K, about 40% of the cycles pre-ignite with nearly all cycles undergoing pre-ignition for temperatures exceeding 1174 K. However, in stark contrast to the early injection timing cases discussed previously, the timing of pre-ignition onset displays a much smaller spread of nominally around ~10-30 CAD centered at around ~300 CAD, i.e., the onset of pre-ignition appears to be less stochastic with glow-plug temperatures seemingly not affecting this trend. This indicates a more repeatable flow and formation of mixture near the glow-plug when the injection timing is delayed from the BDC.

For an SOI of 270 CAD, the timing of pre-ignition onset tends to show a bifurcation, with the pre-ignition timings typically clustered at ~310 CAD (during the compression stroke) for temperatures exceeding 1198 K and at ~440 CAD (during the expansion stroke) for temperatures below 1162 K. Temperature of 1186 K appears to be transition temperature with cycles equally split between the two pre-ignition timings. The pre-ignition onset during the expansion stroke can be in part attributed to the reduced residence time available during the final stages of the compression stroke when the injection timing is late, which necessitates higher glow-plug temperatures to facilitate early pre-ignition before TDC under such conditions.

For the latest injection timing, i.e., SOI = 300 CAD, much higher glow-plug temperatures (exceeding 1198 K) are needed to induce any pre-ignition, though nearly all cycles appear to pre-ignite at these temperature i.e., much smaller temperature rise is required to cause the transition from no pre-ignitions to nearly all cycles undergoing pre-ignition. This trend again seems to support the hypothesis that at later injection timings, the mixture has less residence time near the glow-plug, which reduces the possibility of pre-ignition to occur. In addition, the increased turbulence induced by a late injection can potentially further delay the onset of pre-ignition by reducing the mixture residence time in the direct vicinity of glow-plug. An increased spread in the timing of pre-ignition onset along with the previously noted temperature bifurcation effect is again readily apparent.

FIGURE 6 OH* chemiluminescence based pre-ignition timing and frequency (50 cycles in total) for late injection timings at 1200 RPM for different hot-spot temperatures. Start of injection is 240 CAD (top), 270 CAD (middle) and 300 CAD (bottom). Secondary axis indicates the corresponding cylinder pressure for the indicated CAD timings.

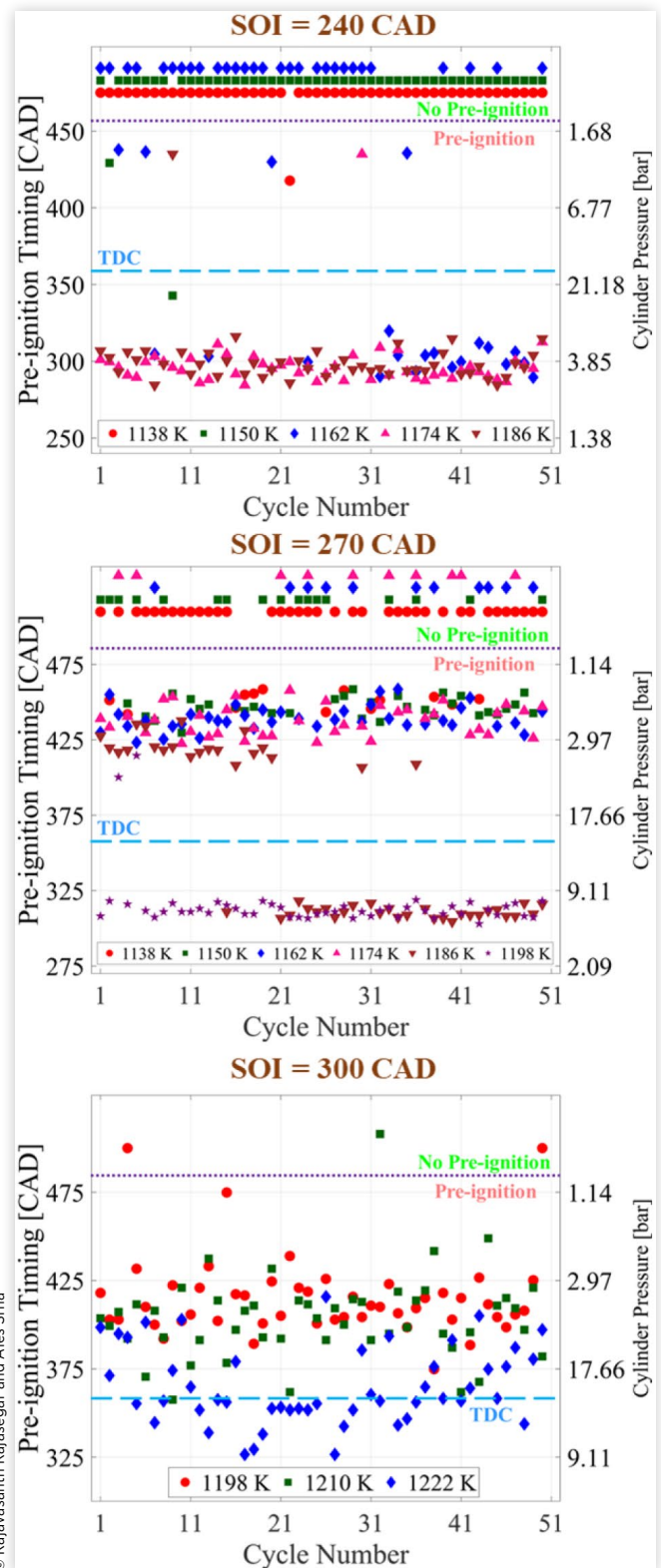


Figure 7 summarizes the information presented across various panels of Figure 5 and Figure 6. The top panel shows the performed glow-plug temperature and injection timing sweep at 1200 RPM, with the red markers at each SOI indicating the percentage of cycles that pre-ignited under each condition tested. This graph clearly shows the sensitivity of pre-ignition frequency to the hot-spot temperature for various injection timings. The middle panel shows the interpolated trend based on the data spanning across the investigated range of injection timings, with the blue shaded area indicating the transition region where between 5% and 50% of the cycles undergo pre-ignition. For very early injection timings (injections during the early intake stroke), this region is relatively narrow which suggests a high sensitivity of the pre-ignition frequency to hot-spot temperature. As the injection is delayed, this region widens, until a threshold injection timing of about ~250 CAD, beyond which it becomes very narrow. This signifies that for late injections (injections during the later part of the compression stroke), the dependence of pre-ignition frequency on the glow-plug temperature is again extremely high.

A very similar behavior is also observable at 600 RPM as shown in the bottom panel of Figure 7. Remarkably, the temperature transition zone marked by the blue shaded area between few-to-no pre-ignition events to over 70% of cycles pre-igniting is even narrower. Under these conditions, only a 10-15 K change in surface temperature of the glow-plug (about 1% absolute temperature change) can transition the engine from stable operation with no pre-ignition to a state, where the majority of cycles are pre-igniting, over a wide range of injection timings. This observed sensitivity is in line with previous investigations on hydrocarbon fuels carried out by Yu et al. [44]

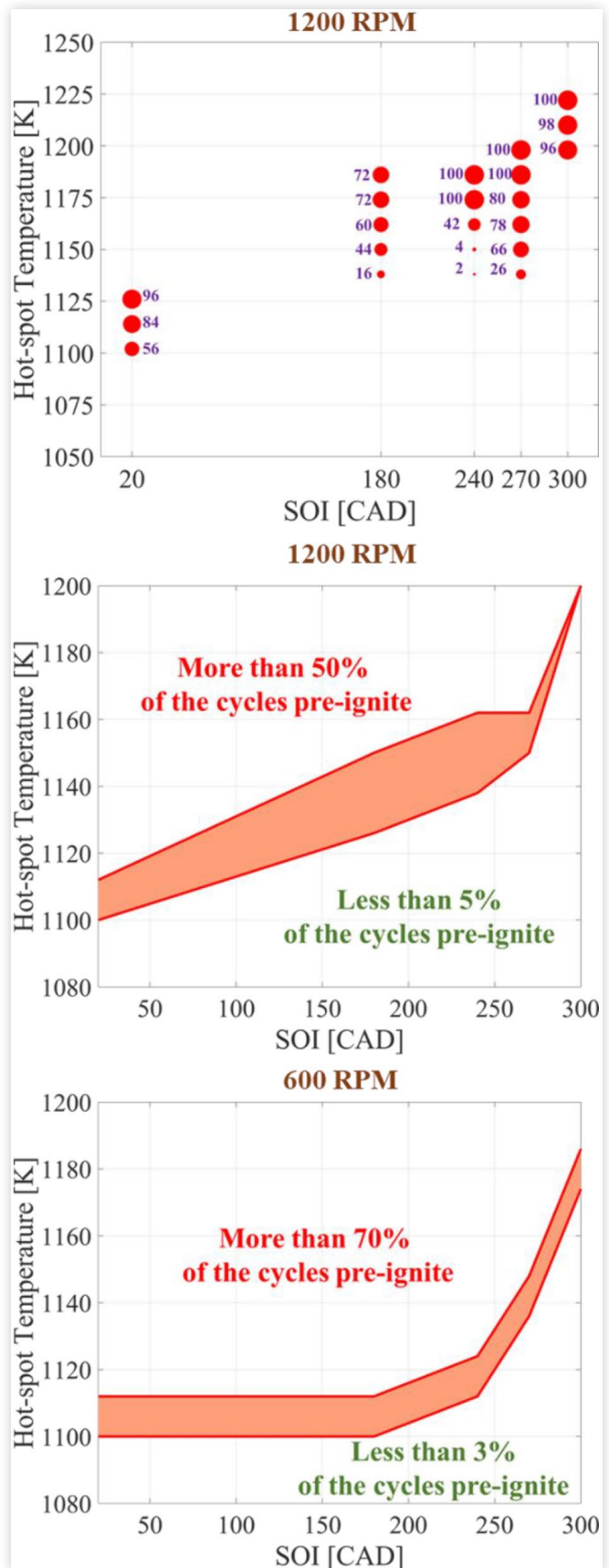
Two potential phenomena could possibly explain this sensitivity: A short residence time of the gases in hot zones induced by the glow-plug, or surface chemistry reactions initiated on the ceramic glow-plug that contribute to pre-ignition, which are only activated above a certain temperature threshold (catalytic reactions). Nevertheless, these arguments need to be further explored in future investigations to fully understand the underlying physico-chemical phenomenon that drives hot-spot induced pre-ignition.

Understanding the Phenomenology of Hot-Spot Induced Pre-Ignition using Fuel Tracer-Plif and O-D Well-Stirred Reactor Chemical Kinetics Simulations

Two major questions still remain from the analysis carried out earlier: Why is the behavior of the timing of pre-ignition onset so stochastic i.e., less predictable at some injection timings? And what is the mechanism behind the bifurcation of pre-ignition timing and the observed sensitivity of pre-ignition to glow-plug temperature?

The first question can potentially be addressed by trying to understand the variability in mixture distribution around

FIGURE 7 Sensitivity of pre-ignition frequency to hot-spot temperature for various injection timings at 1200 RPM (top and middle) and 600 RPM (bottom).



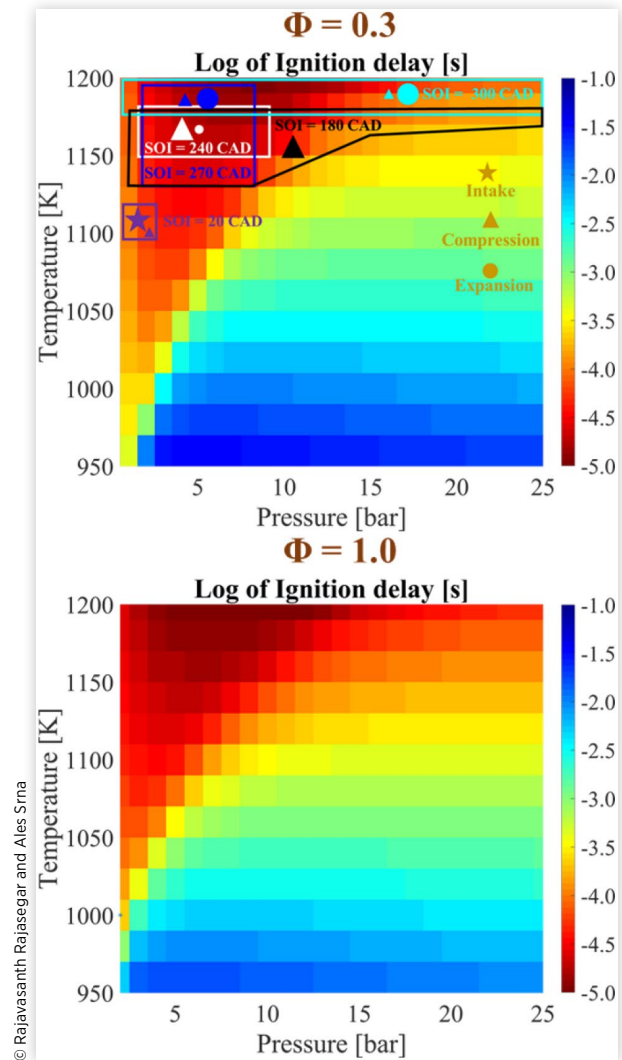
the vicinity of the glow-plug that directly tends to impact the timing of pre-ignition onset and the associated spread. To address this issue, the characterization of mixture distribution near the glow-plug at the time of pre-ignition onset was investigated using the fuel-tracer PLIF method as discussed in the experimental overview section. An engine speed of 1200 RPM and an early injection timing (SOI = 180 CAD) was chosen for this study. The glow-plug was disabled for these tests in order to avoid temperature stratification near the glow-plug. A previous investigation carried out on H₂ direct-injection in this optical engine [42] showed that the fuel-air mixture formed under these operating conditions is quite homogeneous close to the TDC. However, the onset of pre-ignition tends to occur much earlier in the compression stroke under such early injection timing. Thus, based on the estimated timing of pre-ignition onset as shown in Figure 5, the fuel-tracer PLIF images were acquired at 290 CAD to study the mixture stratification and repeatability.

Figure 8 shows the distribution of fuel-air near the vicinity of the glow-plug acquired at 290 CAD for 5 consecutive cycles. From the snapshots, it is clear that the mixture distribution near the glow-plug is indeed very stratified with mixture equivalence ratios ranging from 0 to 0.35 at the time of pre-ignition. Typically, under these conditions, it appears that the immediate vicinity of the glow plug is usually surrounded by ultra-lean mixtures, and given that the chemical reactions can only be initiated after the mixture enters the hot zone, this mixing process is likely to determine the earliest possible timing for onset of pre-ignition due to the location of hot-spot. Furthermore, the cycle-to-cycle variability in the mixture distribution appears to be contributing at least in part to the stochastic nature of the timing of pre-ignition onset that was observed at early injection timings.

To address the second question, we turned our attention to chemical kinetics of hydrogen ignition. A set of 0-D, closed homogeneous reactor (CHR) calculations were performed using CHEMKIN to estimate the ignition delay using the chemical kinetics mechanism for hydrogen oxidation from Conaire et al. [45]. For a comprehensive sweep of engine relevant temperature and pressure conditions, the ignition delay of H₂ was computed for two different equivalence ratios ($\phi = 0.3$ and $\phi = 1.0$) of the fuel-air mixture.

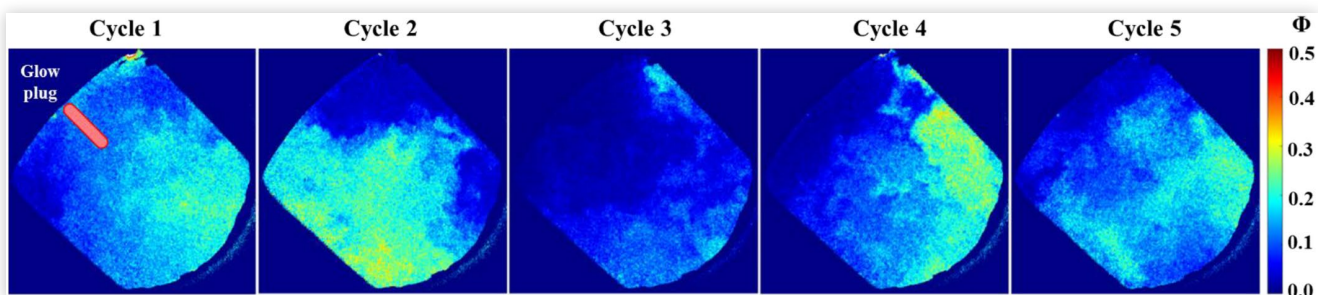
Figure 9 presents the results of CHEMKIN simulations in the form of contour plot with the contours representing the logarithm of the computed ignition delay for two hydrogen fuel-air mixtures namely, $\phi = 0.3$ and 1.0 in the top and bottom

FIGURE 9 Contour plots showing the logarithm of the ignition delay based on 0-D CHR CHEMKIN simulations for two different equivalence ratios ($\phi = 0.3$ -top and $\phi = 1.0$ -bottom) of H₂ fuel-air mixtures for a range of engine relevant pressures and temperatures. The temperature and pressure range for the experimentally observed pre-ignition events for different injection timings are also highlighted. The different markers indicate the timing of the pre-ignition event while the size of the markers indicate the relative frequencies of pre-ignition timings.



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FIGURE 8 Snapshots of tracer-PLIF images showing the distribution of H₂-air mixture near the glow-plug across 5 different cycles. Images were acquired at 290 CAD for an SOI of 180 CAD at 1200 RPM.



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panels, respectively. Each pixel corresponds to the ignition delay calculated at specific temperature and pressure combination – the plots therefore summarize the ignition delay dependence over a wide range of operating pressures and temperatures. Regions of temperature and pressure where pre-ignition was observed experimentally for different injection timings are also overlaid on the simulation results. It is to be noted that this assumes homogeneity of hydrogen-air mixture regardless of the injection timing. The timing of pre-ignition events in the demarcated regions i.e., during intake, compression or expansion stroke is indicated by various markers. The relative size of these markers within a region gives an estimate of the relative frequency of pre-ignition timings.

These simulations reveal that at a given temperature, the ignition delay of hydrogen sharply increases with increasing pressure, which is opposite to the general trend observed with typical hydro-carbon fuels. Thus, at low pressure conditions, the ignition delays tend to be much shorter thereby only needing much lower temperatures to cause ignition. This to some extent explains the tendency of hydrogen to pre-ignite either during the intake stroke or during the early part of the compression stroke. However, as the pressure builds up during the compression stroke, significant enhancement in the ignition delay suppresses the pre-ignition reactions of hydrogen. This explains why the fuel-air mixtures failed to ignite at lower hot-spot temperatures for late injection timings, and why ignition in the expansion stroke at reduced pressure was sometimes observed at those conditions. It can be clearly seen the distribution of the demarcated regions of temperature and pressure where pre-ignition was observed experimentally, closely follows the regions where the computed ignition delay is relatively short.

Furthermore, this behavior seems to be fairly independent of the mixture distribution as indicated by the similar trends observed for the two equivalence ratios that were analyzed. In general, hydrogen seems to exhibit a fairly low sensitivity in terms of the dependence of ignition delay values on fuel-air equivalence ratio.

This behavior highlights a potential mitigation technique to minimize hot-spot induced hydrogen pre-ignition. Operating the engine with boosted intake pressures coupled with later injection timing during the compression stroke can considerably reduce the pre-ignition tendency, as long as the mixing process is sufficiently fast to ensure favorable combustion phasing and low emissions. Nevertheless, further research is needed to develop injection system designs that can support such pre-ignition operating strategies without causing excessive fuel stratification that would result in high engine NOX emissions. Furthermore, hot-spot pre-ignition is just one potential pre-ignition mechanism – research of other mechanisms is equally important to allow efficient mitigation at specific operating conditions of each engine.

Summary and Conclusion

In this work, an experimental study was carried out to characterize hot-spot induced pre-ignition in a direct-injection hydrogen-fueled, heavy-duty, single-cylinder optical engine.

An electrically heated, temperature-controllable, diesel glow-plug was used to create a simulated hot-spot to induce pre-ignition. Experiments were carried out at two different engine speeds for several injection timings for a range of glow-plug temperatures as determined by the applied excitation voltage. IR imaging was used to characterize the surface temperature of the glow-plug based on pre-calibration using a thin wire thermocouple. High-speed OH* chemiluminescence imaging was used in conjunction with cylinder pressure measurements to characterize the timing of pre-ignition onset while the mixture distribution around the glow-plug was characterized by fuel-tracer PLIF. Experimental results were also complemented with 0-D, CHR CHEMKIN simulations to provide further insight about pre-ignition and the impact of temperature and pressure.

The results provide a fundamental understanding on the phenomenology and the underlying physics of the hot-spot induced pre-ignition of hydrogen in SI engines. Based on the results, some potential mitigation strategies aimed to minimize pre-ignition during actual engine operation are also inferred.

Analysis of the experimental results supports the following conclusions:

1. Hot-spot induced pre-ignition requires relatively high glow-plug temperatures (exceeding 1100 K) for all injection timings. However, during the engine operation, since it is quite unlikely that any of the engine components will reach such high temperatures, it is conceivable that pre-ignition of hydrogen will most likely be due to hot-spots localized to crevices or to other pre-ignition sources such as oil droplets or hot-residual gases and un-scavenged particulates from incomplete scavenging.
2. The timing of pre-ignition onset presents a highly stochastic behavior for both early and late injection timings. This is most likely associated with the mixing process — At later injection timings, the mixture has less time to “form” around the vicinity of the glow plug thereby leading to fairly short residence times in the high-temperature regions surrounding the glow-plug.
3. In general, the sensitivity of pre-ignition frequency to the hot-spot temperature is high irrespective of the injection timing. At 1200 RPM, a 20 -30 K increase in the glow-plug temperature was sufficient to increase the number of cycles that pre-ignited from less than 5% to over 50%. This threshold was even lower when considering late injection timings (SOI > 270 CAD) and lower engine speeds (600 RPM), where only a 15 K rise in surface temperature was enough to induce pre-ignition in over 70% of the cycles. This indicates that surface-chemistry reactions in addition to other pre-ignition sources may potentially play an important role in the pre-ignition process of hydrogen which lead to the hypothesis that catalytic surfaces may indeed lower the required temperature for pre-ignition (not tested in this work).
4. 0-D CHR CHEMKIN simulations indicated that the ignition delay of hydrogen sharply increases at elevated pressures, which explains the observed

tendency of the fuel-air mixture to pre-ignite during the intake stroke or early during the compression stroke. Thus, a promising approach to avoid hot-spot induced pre-ignition would be to operate the engine at boosted intake pressures (turbocharging or supercharging) in addition to the use of late injection timing strategies (late during the compression stroke), as long as an optimal compromise is found so as to avoid any undesirable fuel stratification that can potentially lead to increased exhaust emissions.

This study has paved a path for future research to focus on further addressing the challenges associated with the use of hydrogen in SI engines. On this note, some potential future work might include higher-resolution flame and temperature stratification imaging complemented with high-fidelity computational studies to gain further insight into the role of boundary layer thickness, residence time and in-cylinder flow on the hot-spot induced pre-ignition, as well as the potential role of surface-chemistry catalysis-like reactions. The latter study can be carried out by coating the hot-spot with catalytically active metals such as platinum and iridium which are commonly found in spark-plug electrodes. Other potential studies could focus on characterizing different H₂ pre-ignition mechanisms by isolating the source. This could entail an investigation of induced pre-ignition due to controlled oil droplets or combustion residuals (hot internal EGR) as potential sources.

Contact Information

Rajavasanth Rajasegar: rrajase@sandia.gov

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Definitions, Acronyms, Abbreviations

CO₂ - Carbon-di-Oxide

NO_x - Nitrogen oxides

NG - Natural gas

H₂ - Hydrogen

CHP - Combined heat and power

CHR - Closed homogeneous reactor

ICE - Internal combustion engine

OEM - Original equipment manufacturer

FCEV - Fuel cell electric-vehicle

SI - Spark ignition

GDI - Gasoline direct injection

DI - Direct injection

IVC - Intake Valve Closed

IVO - Intake Valve Open

EVC - Exhaust Valve Closed

EVO - Exhaust Valve Open

PLIF - Planar Laser Induced Fluorescence

IR - Infrared

UV - Ultraviolet

BPF - Band pass filter

ICCD - Intensified Charged Coupled Device

°CA - Degrees crank angle (interval/duration)

CAD - Crank-angle degrees (timing)

TDC - Top dead center

BDC - Bottom dead center

RPM - Revolutions per minute

CCV - Cycle-to-cycle variation

SOI - Start of injection

SSE - Start of solenoid energization

ϕ - Relative fuel-air equivalence ratio

λ - Relative air-fuel equivalence ratio

EGR - Exhaust gas recirculation