Ignition Behavior of Hydrogen in the Presence of Lube Oil Behind Reflected Shock Waves

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1 Introduction

The need for reducing greenhouse gas emissions and transition to sustainable energy sources has reignited interest in hydrogen internal combustion engines (H2ICEs). Hydrogen offers several compelling advantages, including high energy density, rapid flame speed, and zero carbon emissions, making it a promising alternative to fossil fuels for mobility and energy applications. However, the unique properties of hydrogen, such as its low ignition energy and wide flammability range, pose significant challenges for internal combustion engine design and operation. Among these challenges are abnormal combustion phenomena, including pre-ignition and knock, which can compromise engine performance, efficiency, and durability [1]. Overcoming these challenges requires advancements in fuel injection strategies, thermal management systems, and combustion modeling to ensure efficient and reliable hydrogen utilization. One critical yet underexplored factor influencing hydrogen combustion is the role of lubricant oil. Studies have shown that lubricant oil can act as a precursor for abnormal combustion events due to its low auto-ignition resistance and complex chemical composition. The presence of lubricant oil can significantly alter the ignition delay time (IDT) of hydrogen, especially at low and intermediate temperatures common during engine operation [2].

Lubricant oil can inadvertently enter the combustion chamber through various routes, such as piston ring blow-by, valve stem seals, or injector systems, where it interacts with the fuel-air mixture. In two-stroke engines, scavenging—a process essential for removing exhaust gases and introducing fresh air-fuel mixtures—can also carry oil droplets into the combustion chamber. The degradation of the oil film on cylinder walls, exacerbated by high pressures, temperatures, and piston motion, further contributes to oil entrainment. These oil droplets or vapors can create localized fuel-rich regions, increasing the likelihood of premature ignition and, consequently, engine knock or mechanical failure [3,4]. Research indicates that lubricant oil droplets can also originate from the crankcase, where the action of rotating components like the crankshaft and connecting rods contributes to the atomization of oil. Droplet sizes, ranging from 10 μm to 3 mm [5,6], can impact combustion dynamics significantly. When these droplets vaporize and ignite prematurely, they disrupt controlled combustion by causing early flame propagation, leading to abnormal rises in in-cylinder pressure and temperature. These conditions not only reduce engine efficiency but also increase wear and tear on engine components, resulting in higher maintenance costs and shorter engine lifespans. Understanding these mechanisms is crucial for developing strategies to improve the performance and durability of hydrogen-based engines.

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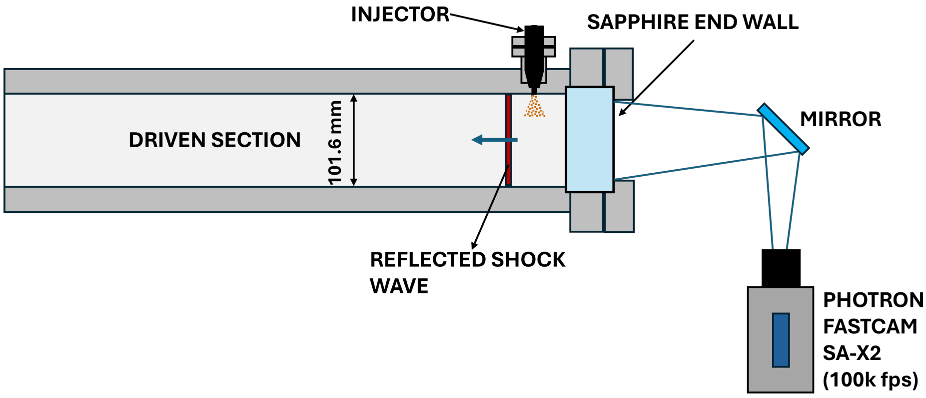

Figure 1: Experimental setup for showing the end wall imaging setup in the HPST and the mounting of the injector to introduce lube oil behind the reflected shock wave.

The present study aims to address this gap by investigating the effects of lubricant oil under engine-relevant conditions through shock tube experiments. These experiments are conducted with hydrogen-air mixtures and a lubricant oil surrogate, n-hexadecane (n-$C_{16}H_{34}$). The hydrocarbon structure of n-$C_{16}H_{34}$, characterized by its linear configuration and numerous secondary C-H bonds, makes it highly reactive to hydrogen abstraction, even at lower temperatures. This reactivity plays a significant role in influencing the pre-ignition behavior of hydrogen-air mixtures. Advanced diagnostic techniques, including high-speed imaging and pressure measurements near the shock tube end wall, are employed to capture detailed ignition dynamics. By analyzing ignition delay times, flame propagation, and heat release characteristics, this study aims to quantify the impact of lubricant oil on hydrogen combustion stability and efficiency. The findings will provide valuable insights for optimizing lubricant formulations and engine designs to minimize abnormal combustion phenomena, paving the way for the reliable and sustainable operation of hydrogen internal combustion engines.

2 Experimental Methodology

Experiments have been conducted in the high-pressure shock tube (HPST) facility at KAUST. Figure 1 shows the modifications made near the end of the shock tube to facilitate high-speed imaging and injection of the lube oil. An optical quality sapphire end wall is used to enable viewing of the entire cross-section of the shock tube. A piezo-controlled injector (Model: HDEV-4, Robert Bosch GmbH, Germany) is mounted on the side wall close to the end of the shock tube to inject the lube oil. This injector is suitable for the present work as it possesses several features that align well with the current requirements. It can handle injection pressures of up to 200 bar, allowing for a robust delivery of fluids and the duration of injection can be varied over a wide range, from 70 to 4000 μs, providing flexibility in how quickly the oil or surrogate is introduced. The needle lift can also be adjusted from 0 to 180 volts, further enhancing control over the injection process. Experiments are targeted in the low-to-intermediate temperature regime, specifically between 970 K and 1150 K. This temperature range has been shown to exhibit higher reactivity for lubricant oil surrogate (n-$C_{16}H_{34}$) species compared to hydrogen, particularly within a pressure range of 10 to 60 bar [5].

The lubricant oil injection strategy is designed to precisely introduce oil or n-hexadecane droplets into the shock-heated region, specifically within the P_5 and T_5 reflected shock zones. In a typical experiment for this study, H_2-air mixture is used in the driven section of the shock tube. High-pressure helium or mixture of helium and nitrogen (in case of tailoring to obtain longer test times) is used as the driver gas.

Upon rupture of the diaphragm placed between the driver and the driven gas, an incident shock wave propagates through the driven gas mixture. The lube oil injection system is triggered by a pressure sensor installed at 2 cm upstream of the end wall. This sensor detects the pressure rise caused by the reflected shock wave. Upon detection, a function generator sends a Transistor-Transistor Logic (TTL) pulse to the injector control unit, which generates the desired pulse shape for the injector. This sequence ensures precise injection of the lube oil into the high-temperature and high-pressure region behind the reflected shock wave, as illustrated in Figure 1. Ignition delay times (IDTs) are obtained by monitoring the pressure profile using a sensor (Model: 112B05, PCB Piezotronics Inc., USA) mounted on the side wall at a location 2 cm from the shock tube's end. Detailed methodology of extracting IDTs from the pressure traces are well documented elsewhere [7]. Experimental IDTs are compared with zero-dimensional (0-D) constant volume simulations conducted in CHEMKIN Pro 2022. For these comparisons, the FFCM v1.0 mechanism [8] is employed to evaluate the IDTs of pure-H_2 mixtures.

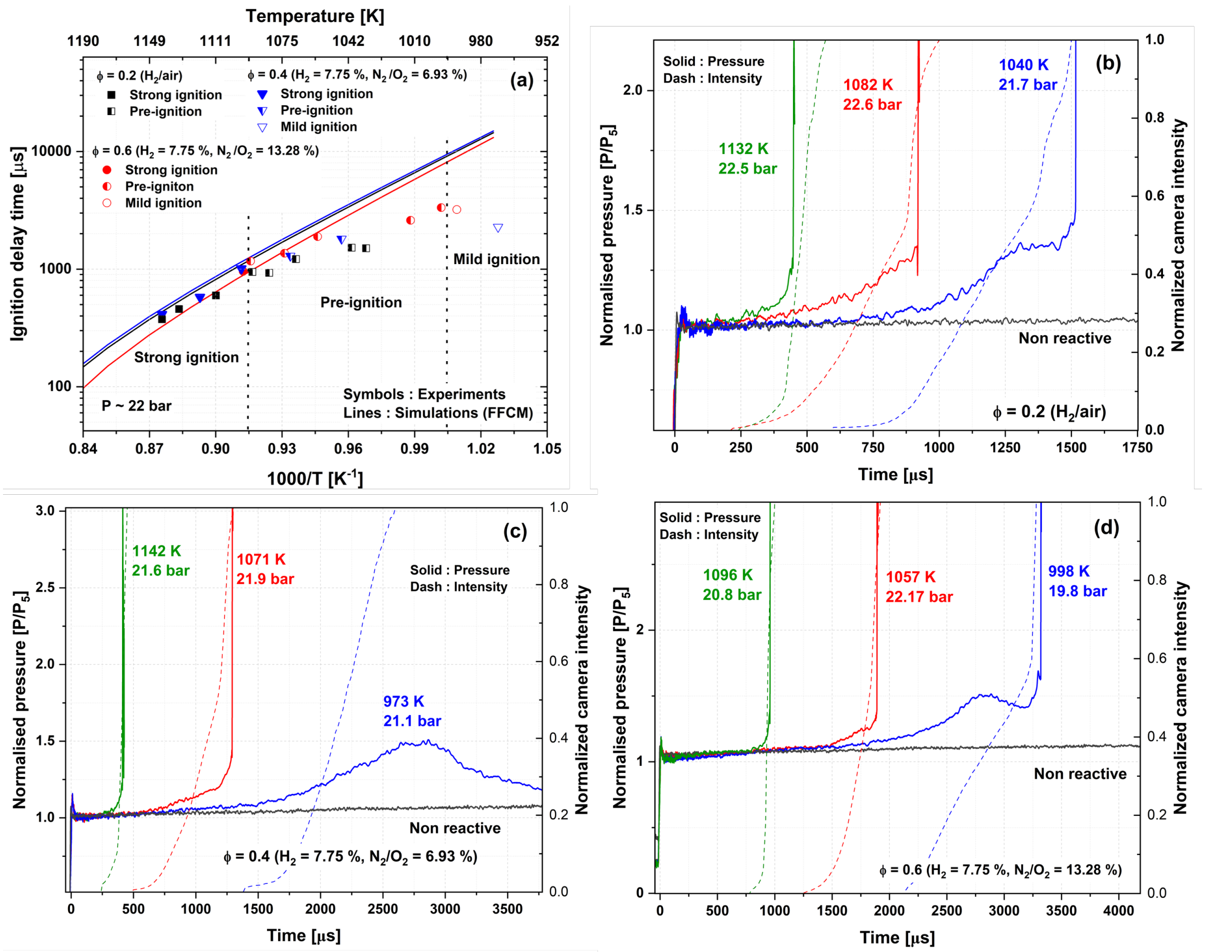

Figure 2: (a) Variation of IDTs with temperature for hydrogen in air and diluted mixtures at 22 bar. Simulations were performed with Chemkin using FFCM mechanism. Comparison of normalized pressure time histories at 22 bar (solid line) and normalized camera intensities (dotted line). (b) H_2/air mixture at temperature between 1140 K and 1040 K. (c) H_2 (7.75%)-N_2/O_2 (6.93%) mixture at temperature between 1150 K and 970 K. (d) H_2 (7.75%)-N_2/O_2 (13.28%) mixture at temperature between 1100 K and 990 K. The pressure history for non-reactive mixture is also provided as a reference.

3 Results and Discussion

Initially, experiments were performed using H_2 mixtures without the presence of lube oil in the high-pressure shock tube. These baseline experiments served as a reference for comparison with cases involving lube oil injection and provided insights into the fundamental ignition regimes of H_2 mixtures under controlled conditions. High-speed imaging diagnostics were incorporated to detect any non-idealities in the behavior of H_2 mixtures, ensuring the accurate characterization of ignition phenomena. IDTs for the equivalence ratio range $\phi = 0.2 - 0.6$ are shown in Fig. 2a as scatter points, with corresponding 0-D simulation predictions from the FFCM kinetic model represented by solid lines. The IDTs exhibit minimal dependence on ϕ, a behavior attributed to the consistent mole fraction of H_2 across all tested equivalence ratios. This experimental design, which maintains a uniform H_2 mole fraction while varying O_2 to adjust ϕ, is supported by existing literature [9], which highlights the potential for extreme non-ideal ignition behaviors in H_2/air mixtures within this equivalence ratio range. Figure 2a also reveals occurrences of pre-ignition (indicated by half-filled symbols) and mild ignition (indicated by hollow symbols) at lower temperatures for all tested mixtures. These non-ideal ignition behaviors are further illustrated in the pressure traces shown in Figs. 2b-d. Cases of strong ignition (depicted in green) exhibit an abrupt and well-defined pressure rise characteristic of homogeneous ignition. In contrast, pre-ignition cases (in red) display a gradual pressure increase preceding a sharp jump, indicative of localized ignition events triggering global ignition. Mild ignition cases (in blue) exhibit a unique behavior, with a gradual pressure rise followed by a temporary drop before transitioning into a sharp pressure increase. These distinctions provide critical insights into the underlying mechanisms governing ignition behavior in H_2 mixtures.

To further elucidate the nature of ignition events, high-speed images captured from the shock tube end wall are presented in Fig. 3 for three different temperatures. These images, annotated with timestamps corresponding to moments just before the main ignition, provide visual evidence of the ignition dynamics. At the highest temperature (1096 K, shown in 3a), ignition appears predominantly homogeneous, with minor signs of pre-ignition visible in the lower-right corner. This pre-ignition swiftly transitions into global ignition within tens of microseconds. At lower temperatures, particularly at 998 K (Fig. 3c), emissions indicative of pre-ignition are observed as early as 1 ms prior to the main ignition event. These emissions progressively intensify, eventually encompassing the entire mixture and culminating in global ignition. To correlate the onset of pressure rises due to pre-ignition with emissions captured in the high-speed images, normalized camera intensity profiles are plotted alongside pressure data in Figs. 2b - d. A consistent pattern emerges: in strong ignition cases, the sharp rise in camera intensity coincides with the abrupt pressure increase. Conversely, for pre-ignition and mild ignition cases, the gradual increase in camera intensity aligns closely with the pressure trend, reflecting the slower and spatially localized ignition dynamics before the eventual global ignition. These observations highlight the susceptibility of pure H_2 mixtures to non-ideal ignition phenomena within the shock tube, underscoring the critical need to identify temperature ranges where such effects are minimized. This understanding is essential for ensuring that subsequent experiments involving lube oil injection in H_2 mixtures yield reliable and reproducible IDT data.

Preliminary results of experiments which had lube oil surrogate injection is illustrated in Fig. 4. While the actual injection event is not clearly visible due to insufficient lighting and high-speed dynamics, the effects become evident approximately 300 μsecs prior to the main ignition. At this point, isolated droplet ignition is observed, marked by localized luminous emissions. This droplet ignition represents the initial interaction between the oil and the surrounding high-temperature H_2-O_2 mixture, highlighting the role of the lube oil as a secondary ignition source. Following this initial ignition, hot spots are observed near the base of the shock tube that could be due to diaphragm particles that become more prominent as time progresses and accelerates the combustion process. At 20 μsecs before the main ignition, a

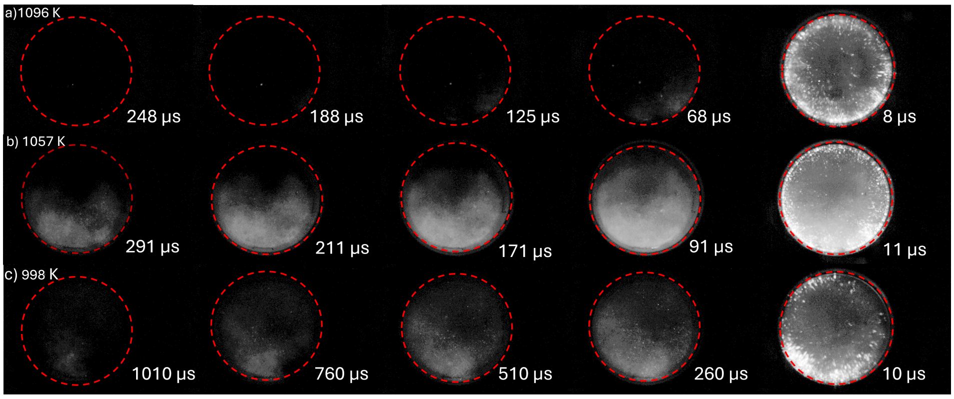

Figure 3: End wall visualization for the H_2 (7.75 %)-N_2/O_2 (13.28 %) mixture at different temperatures. (a) T_5 = 1096 K. (b) T_5 = 1057 K. (c) T_5 = 998 K. The time mentioned in the figure shows the time before the main ignition.

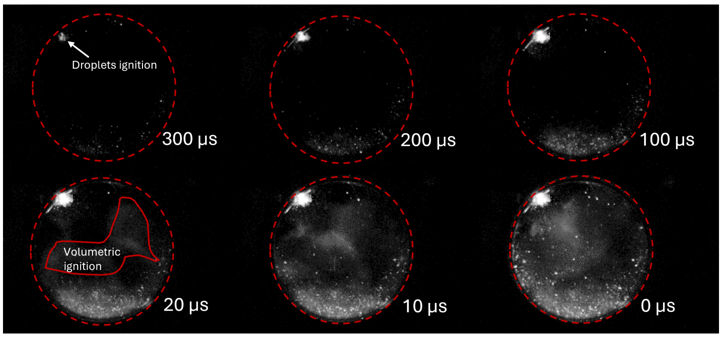

Figure 4: Injection of lube oil surrogate (n-hexadecane) droplets in H_2 (7.75 %)-N_2/O_2 (6.93 %) mixture at T_5 = 1091 K and P_5 = 22.2 bar. The injector was triggered by the reflected shock pressure signal. The injection pressure was maintained by a pump at 24.5 bar. The time indicated against each image is the time before the main ignition event corresponding to the rise in the pressure profile.

distinct volumetric ignition event occurs, characterized by the rapid and nearly simultaneous ignition of the remaining unburned mixture. This transition to volumetric ignition is evident in the high-speed images, where the flame front evolves into a more uniform and intense luminosity, indicating complete combustion. In this specific experiment, the influence of lube oil surrogate droplets on the overall ignition process appears to be minimal, primarily because of the inherently short ignition delay time of the H_2-O_2 mixture under the tested conditions. The rapid ignition dynamics of the hydrogen-based mixture leave little time for the oil-induced flame to significantly alter the combustion process. Future experiments will target lower temperatures, where longer IDTs allow the flame initiated by the lube oil surrogate to propagate further and may trigger an earlier volumetric ignition event.

4 Summary and Future Work

The present study explores the effect of lube oil droplets on the ignition behavior of hydrogen mixtures relevant to their use in H2ICEs. Experiments are performed initially to capture the different regimes of ignition namely, mild, strong and pre-ignition cases in hydrogen mixtures. High-speed imaging and the pressure traces obtained near the end wall provides insights into these ignition regimes. Preliminary experiments of lube oil droplets injection at higher temperatures show that the ignition initiated by the lube oil does not affect the global strong ignition of the hydrogen mixture. Future work will focus on exploring these scenarios at lower temperatures, where the interaction between lubricant oil droplets and the H_2-O_2 mixture is expected to have a more pronounced impact on the ignition behavior. By systematically varying the temperature and equivalence ratio, and using advanced diagnostics to capture the spatial and temporal evolution of ignition, these studies aim to quantify the extent to which lubricant oil affects ignition timing, flame propagation, and combustion dynamics.

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