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Experimental analysis of the effect of end-gas temperature on spontaneous detonation development mechanisms for a hydrogen/n-decane mixture

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Abstract

Constant Volume Combustion (CVC) is a Pressure Gain Combustion technology which is based on the Humphrey thermo-dynamic cycle. In CVC and wider combustion applications, unwanted transitions to detonations can occur in highly reactive end-gas. In the present work, the difference in combustion regimes when changing the initial temperature gradient for stoichiometric 5% H₂/C₁₀H₂₂/O₂/Ar mixtures was explored. Different temperature gradients were imposed on the reactive gaseous mixtures in a closed optical vessel through varying the temperature of heating cartridges throughout the chamber. Ultra-high-speed cameras were used to capture and analyze the resulting combustion regimes. Transitions to detonation through multiple mechanisms were observed. It was found that when the reactive end gas has temperatures near the boundary of the Negative Temperature Coefficient (NTC) region, a difference in temperature of just a few Kelvin can greatly change the mechanism by which a detonation develops.

Keywords: *Autoignition, Transition, Detonation*

1. Introduction

Pressure Gain Combustion (PGC) is a type of combustion technology where a net increase in stagnation pressure is enabled by allowing gas expansion and heat release in a constrained environment. PGC technologies include Constant Volume Combustion (CVC) which is based on the Humphrey thermo-dynamic cycle and can potentially lead to an efficiency gain of up to 20% [1].

In CVC and other combustion applications where the end gas can become very reactive, unwanted transitions to detonations can occur through different mechanisms, one of which is the Deflagration-Autoignition-Detonation-Transition mechanism (DAIDT). In this mechanism, inhomogeneities in the premixture can lead to spots of increased reactivity (termed hot spots). In reactive end-gas, if there is a reactivity gradient across the hotspot, neighboring pockets of gas can sequentially autoignite which produces an autoignition wave. According to the Shockwave Amplification by Coherent Energy Release (SWACER) model [2], autoignition in a confined space induces pressure waves which propagate ahead into the unburnt gas. If the heat release from the autoignition wave is in phase with these leading pressure waves, the heat release will feed into the pressure waves, reinforce them and lead to a transition to detonation. This is one of the phenomena responsible for super-knock in spark ignition (SI) engines [3].

Outside of DAIDT, there are other detonation transition mechanisms. When numerically simulating a propagating deflagration in a closed vessel, it was observed that in certain conditions, autoignition occurred in the unburnt gas at the end-wall due to the effect of reflected pressure waves [4]. In a Rapid Compression Machine (RCM) configuration, this end wall autoignition led to a mode of detonation transition called

Shockwave Reflection Induced Detonation (SWRID) [5]. In this mechanism, shockwaves reflecting from the chamber walls couple with the heat release from local autoignition and this coupling leads to a detonation developing.

Hydrogen is an attractive fuel for the future because of its zero-carbon emissions. However pure hydrogen is challenging to implement in propulsion applications, therefore mixing hydrogen with jet fuels is a first feasible step towards decarbonization. Linear hydrocarbons are major components of kerosene and can be considered representative of kerosene's behavior but with a much simpler chemical composition and chemistry [6]. N-decane is a large hydrocarbon which experiences 2-stage ignition. The 2nd stage ignition along the reactivity gradient generates a Main Heat Release (MHR) autoignition wave. N-decane also experiences Negative Temperature Coefficient (NTC) behavior. NTC behavior has been found to largely influence the resulting combustion regimes [7][8].

The aim of this present study is to analyze the combustion regimes which occur for stoichiometric hydrogen/n-decane/air mixtures at different temperature gradient conditions in a CVC configuration with end gas temperatures close to the NTC region. Specific attention will be paid to the mechanisms by which detonations develop. These results will act as a first step towards developing strategies to suppress detonations in CVC applications.

2. Methods and Experimental set-up

The Modular Deflagration Autoignition Detonation (MDAID) combustion chamber used in the present work is shown in figure 1d. The combustion chamber has dimensions of 40 x 40 x 172 mm³. Heating cartridges are placed at the top, middle and bottom of the chamber. Each set of heating cartridges are controlled by 3-zone PID regulators. The wall temperature is monitored by thermocouples mechanically fastened into the chamber walls. By setting the PID-regulators to different set-points, a temperature gradient will be imposed on the gas within the chamber. The PID-regulators monitored the wall temperatures. To find the corresponding temperature of the gas within the chamber, the spark plug was replaced with a cap with a K-thermocouple with a 7.6 μm wire diameter mounted to it. The chamber was heated to the experimental configuration, the temperature was taken every 5 mm on a vertical axis between the bottom wall of the chamber (henceforth referred to as the end wall) and 130 mm above the end wall.

A spark plug was mounted at the top wall of the chamber, the chamber was initially filled with the fuel-air premixture. It was found that when a deflagration propagates in a closed tube, due to hydrodynamic processes, an inverted flame front curvature called a tulip flame would eventually form [9] as shown in figures 1a,1b, and 1c. The unburnt gas within this tulip flame pocket is considered to experience conditions comparable to adiabatic compression. The spark plug was ignited delivering an energy discharge of approximately 30 millijoules, the resulting deflagration propagated down the chamber, evolved into a tulip flame and compressed the unburnt gas until the gas was reactive enough to autoignite. The subsequent combustion processes were observed through 40 x 60 mm UV quartz windows located at the bottom of the chamber.

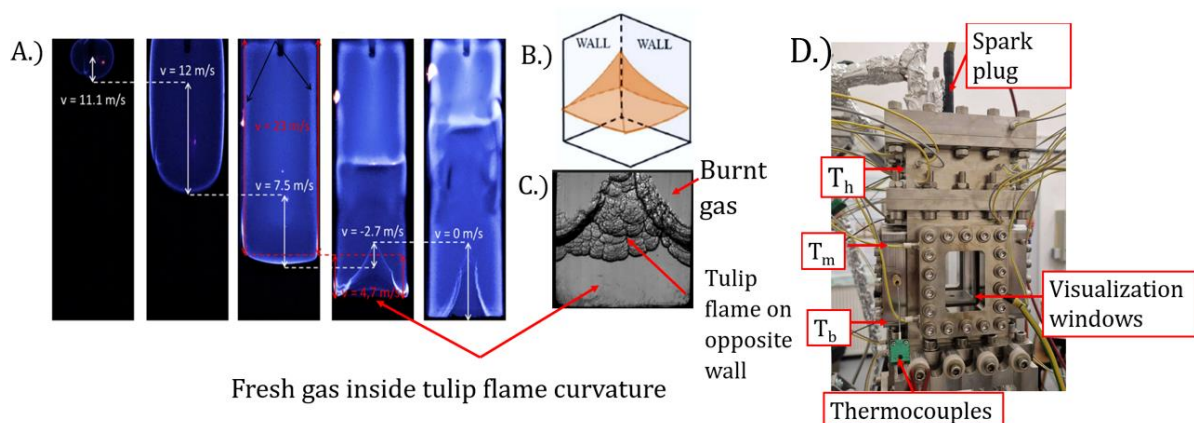
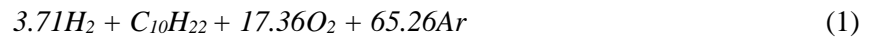


Fig. 1 a.) Example of a tulip flame formation in a 120 mm chamber [21]. The top of the chamber corresponds to the upper chamber wall, b.) A schematic drawing of tulip flame structure [21], c.) A schlieren image of a tulip flame for a stoichiometric $C_{10}H_{22}/O_2/Ar$ mixture, d.) Experimental MDAID chamber used in present study

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Both a high-speed photron SAZ camera with a capture speed of 80,000 frames per seconds and an ultra-high-speed Shimadzu HPVX2 camera with capture speeds of up to 10,000,000 frames per second were used to capture schlieren images of the resulting combustion regimes which usually occurred in the first 45 mm from the end wall of the chamber.

A piezo electric pressure sensor (Kistler 6152CU20) mounted at the end wall monitored the pressure evolution of the chamber at a frequency of 12.5 MHz. In this present work, stoichiometric 5% H₂/C₁₀H₂₂/O₂/Ar mixtures were investigated. The 5% H₂ refers to a fuel mass percentage. Equation 1 shows the composition of the 5% H₂/C₁₀H₂₂/O₂/Ar mixtures.



A 5% H₂ fuel mass percentage corresponds to a 78.8% molar fuel percentage. As the molar composition determines the chemical behavior, this mixture provided a good insight into the effects of mixing hydrogen with n-decane. Argon was chosen for the synthetic air because compared to nitrogen, it has a higher specific heat ratio (γ), a higher temperature is attained for the same compression and it is therefore easier to achieve conditions favorable to autoignition.

A gaseous H₂/O₂/Ar mixture was prepared in a pressurized bottle. Liquid n-decane was injected via a syringe into the vacuumed heated chamber where it immediately vaporized. The increase in the partial pressure was measured by a heated capacitive pressure sensor (MKS baratron 631) with a sensitivity range of 0 – 1300 mbar and a precision of 0.1 mbar. The gaseous mixture bottle was shaken to ensure mixing homogeneity between the low-density hydrogen and synthetic air. The gaseous mixture was then added slowly to the heated chamber to avoid re-condensation of the vaporized n-decane. During the gaseous mixture addition, the overall chamber pressure was measured by a 0-13000 mbar capacitive pressure sensor (MKS baratron 631). The mixture composition was controlled through monitoring the partial pressures. The heated chamber containing the complete premixture was left for 10 minutes to homogenize before the spark plug was ignited. At least 10 experiments were performed for each temperature gradient condition.

2.3 Numerical tools

The temperature evolution of the unburnt gas during the combustion processes could not be measured experimentally and was simulated using a 0-D compressor which simulated autoignition under adiabatic and variable volume conditions by following the experimental pressure evolution. All the numerical tools were built using the Cantera library and the mechanisms selected was the n-decane Polimi mechanism [10].

3. Results and discussion

In all tests, the 5% H₂/C₁₀H₂₂/O₂/Ar mixtures were initially at 3 bar. The temperature of the top heating cartridges (T_h) and the middle heating cartridges (T_m) were set to 453 K and 455 K respectively. The temperature gradient was varied through changing the temperature of the bottom heating cartridges (T_b). T_b values of 433 K, 441 K, 443 K and 445 K were investigated. At least 10 experiments were performed for each heating condition. All observed detonation kernels were confirmed as detonation kernels through verifying that the kernel speed obtained the simulated Chapman Jouguet (CJ) speed.

The compression from the deflagration takes the gas to conditions where it is reactive enough to autoignite. The compressed temperature profile is what will determine the properties of the resulting autoignition waves and subsequent combustion regimes. The 0-D compressor was used to simulate the properties of the gas temperature profile just before autoignition. Table 1 summarizes the percentage of cases resulting in detonation as well as the state II mean chamber conditions for each heating condition. At each condition, the compressed temperatures were found to fall close to the boundary of the NTC region when compared to the simulated constant volume ignition delay time (IDT) values at the compressed pressure. The difference in the initial mean chamber temperature did not significantly vary the deflagration speed, but a higher mean chamber temperature led to a slightly earlier autoignition onset. An earlier autoignition meant that the unburnt gas was subjected to less deflagration compression before the autoignition processes occurred. This is why the mean pressure increases slightly as T_b decreases.

T_b Temperature (K)	Mean initial chamber temperature (K)	Mean compressed chamber temperature (K)	Mean compressed chamber pressure (bar)	Percentage cases transitioning to detonation (%)
433	451	771	17.99	0
441	452	763	17.29	100
443	453	764	17.25	100
445	453	764	17.21	100

Table 1 Mean compressed conditions and percentage of cases transitioning to detonation for 5% H_2 / $C_{10}H_{22}$ / O_2 /Ar mixtures initially at 3 bar.

3.1 Observed combustion regimes

$T_b = 433$ K

Figure 2 shows schlieren images of the MHR propagation regime for the condition where $T_b = 433$ K taken at a capture speed of 80,000 frames per second. As shown in figure 2, an MHR autoignition wave occurred and propagated to the end wall with no transition to detonation.

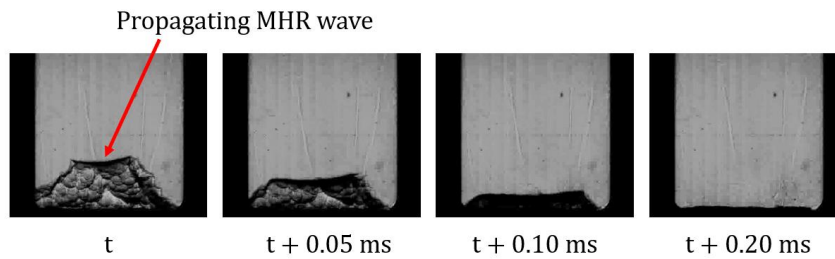


Fig. 2 Schlieren images of combustion regime for a stoichiometric 5% H_2 / $C_{10}H_{22}$ / O_2 /Ar mixture with the heating configuration of $T_h=453$ K, $T_m= 455$ K, $T_b = 433$ K. The mixture is initially at 3 bar and the camera has a capture speed of 80,000 frames per second.

$T_b = 441$ K

Figure 3 shows ultra-high-speed images for the MHR combustion regime for the heating condition where $T_b = 441$ K taken at a capture speed of 500,000 frames per second.

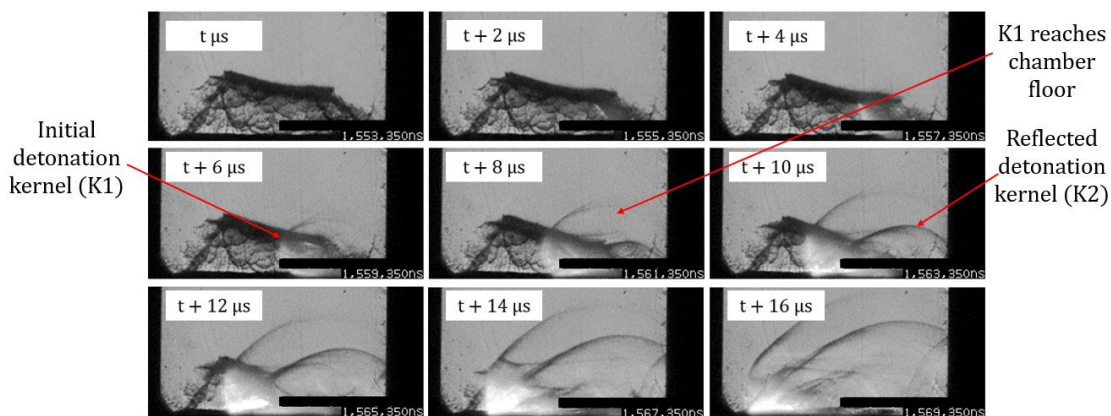


Fig. 3 Schlieren images of the combustion regime for a stoichiometric 5% H_2 / $C_{10}H_{22}$ / O_2 /Ar mixture with the heating configuration of $T_h=453$ K, $T_m= 455$ K, $T_b = 441$ K. The mixture is initially at 3 bar and the camera has a capture speed of 500,000 frames per second.

As shown in figure 3, there is an initial detonation kernel (K1) which originates from the MHR autoignition wave by the MHR wave accelerating and the heat release coupling with pressure waves by the

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DAIDT mechanism described in [11]. This detonation kernel continues to propagate radially outwards until it hits the end wall at a time of $t + 8 \mu\text{s}$. This detonation wave then reflects on the end wall or window edge, leading to a reflected kernel (K2). It was verified that the K2 kernel attained the CJ speed when propagating into the unburnt gas region. Therefore, K2 was a reflected detonation. The K2 kernel goes on to consume the remaining unburnt gas.

$T_b = 443 \text{ K}$

Figure 4 shows the schlieren images of the combustion regime for the heating condition where $T_b = 443 \text{ K}$. The schlieren images were taken by the ultra-high-speed camera at a capture speed of 2,000,000 frames per second. The bottom row of images shows the subtracted images. As shown in figure 4, as the MHR autoignition wave is propagating, a detonation kernel forms at the MHR location (K1) which is consistent with the DAIDT mechanism described in [11]. However, before the kernel K1 starts to form, multiple detonation kernels already start forming at the end wall. Kernel K1 propagates and then eventually reaches the end wall. The detonation kernels originating from the end wall and the reflected detonation kernel all consume the remaining unburnt gas.

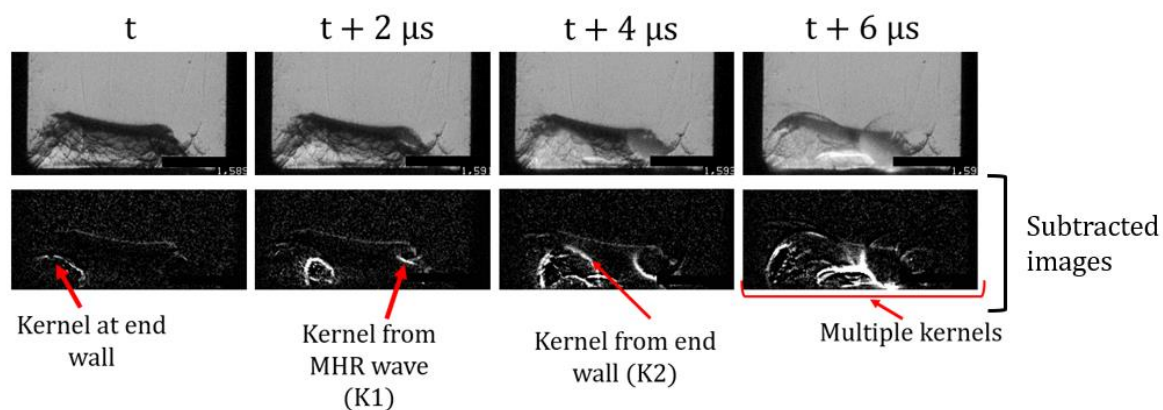


Fig. 4 Schlieren images of the combustion regime for a stoichiometric 5% $\text{H}_2/\text{C}_{10}\text{H}_{22}/\text{O}_2/\text{Ar}$ mixture with the heating configuration of $T_h=453 \text{ K}$, $T_m= 455 \text{ K}$, $T_b = 443 \text{ K}$. The mixture is initially at 3 bar and the camera has a capture speed of 2,000,000 frames per second.

$T_b = 445 \text{ K}$

Figure 5 shows the schlieren images for the combustion regime for the heating condition where $T_b = 445 \text{ K}$.

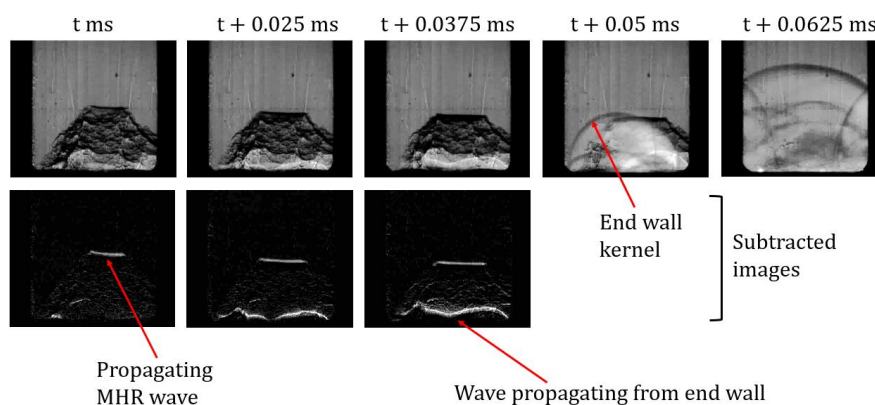


Fig. 5 Schlieren images of the combustion regime for a stoichiometric 5% $\text{H}_2/\text{C}_{10}\text{H}_{22}/\text{O}_2/\text{Ar}$ mixture with the heating configuration of $T_h=453 \text{ K}$, $T_m= 455 \text{ K}$, $T_b= 445 \text{ K}$. The mixture is initially at 3 bar and the camera has a capture speed of 80,000 frames per second.

As shown in figure 5, a wave started to propagate from the end wall. Based on the order of the wave speed, this wave speed was found to be an autoignition wave. As shown in figure 5, at a time of $t + 0.05$ ms, the autoignition wave eventually developed into a detonation kernel which consumed the unburnt gas before a detonation kernel had time to form at the original MHR.

4. Conclusion

In conclusion, this study aimed to explore the difference in combustion regimes when changing the initial temperature gradient for stoichiometric 5% $H_2/C_{10}H_{22}/O_2/Ar$ mixtures. The temperature gradient was varied through varying the temperature of the bottom heating cartridges (T_b). T_b temperatures of 433 K, 441 K, 443 K and 445 K were tested. Ultra-high-speed schlieren images were used to analyze the specific mechanisms by which detonations developed. For all the conditions explored in this present study, the temperature range of the compressed temperature profile of the unburnt gas was close to the NTC boundary. It was observed that at a condition of $T_b = 433$ K, the MHR wave did not transition to detonation. At a condition of $T_b = 441$ K, a detonation kernel formed at the MHR location by the DAIDT mechanism. However, at a condition of $T_b = 443$ K, detonation kernels developed both at the end wall and at the MHR location and at a condition of $T_b = 445$ K, an additional autoignition wave formed at the end wall and propagated up the chamber. This present study demonstrated that for end gas temperatures near the NTC region, a difference in temperature of just a few Kelvin can greatly change the mechanism by which a detonation develops

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