

PREMIXED COMBUSTION OF ACETYLENE-HYDROGEN FUEL MIXTURES FOR THERMODYNAMIC STATE GENERATION IN A CONSTANT VOLUME COMBUSTION VESSEL

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Abstract

Flammability limits and flame speeds of dilute-lean fuel mixtures of hydrogen (H_2) and acetylene (C_2H_2) premixed with oxygen (O_2) and nitrogen (N_2) were examined with a detailed kinetics model. These mixtures are used in a preburn in a constant volume combustion vessel to create elevated temperatures and pressures with gas compositions that represent the thermodynamic state in a diesel engine combustion chamber at fuel injection and autoignition.

A mixture of hydrogen and acetylene with combined atomic hydrogen to carbon ratio (HCR) of 1.85 was used to match that of typical diesel fuel and results are shown in comparison to a previously used mixture with a HCR of 1.17. The lower flammability limit (LFL) of the $HCR_{1.85}$ fuel mixture was found at an equivalence ratio of 0.235, while flame speed and adiabatic combustion temperatures were also predicted for post preburn product oxygen levels between 0 and 21 percent. Flame speeds were shown to decrease with a reduction in oxygen concentration, an increase in nitrogen dilution, while combustion temperatures increased over most of this range. Trends for this relation of flame speed and temperature are presented and a new premixed fuel mixture with an HCR of 1.85 is proposed.

Keywords: combustion engine, diesel engine, combustion processes, pressure vessel, preborn

1. Introduction

Combustion reactants in diesel engines are composed of diesel fuel, fresh air charge, in-cylinder residuals, and recirculated exhaust gas consisting largely of N_2 , O_2 , CO_2 and H_2O . The fractions of these constituents affect spray characteristics, onset of ignition, and the subsequent flame propagation of the combusting diesel fuel during injection [11-13]. Modern diesel engines employ high levels of diluents through exhaust gas recirculation (EGR) [2] or variable valve timing [5] to reduce the oxygen concentration of the combustible mixture. This in-turn reduces flame temperatures and therefore NO_x emissions [2].

A constant volume combustion vessel (CV) with a lean-dilute premixed burn has proven useful for studying diesel sprays and combustion [11-13] with the effects of dilution by matching the thermodynamic conditions observed in an engine, including temperature, pressure, and gas composition. In this process, a premixed charge of gaseous fuels and a variable O_2 and N_2 mixture is ignited and combusted to yield high pressure and temperature conditions characteristic of in-cylinder compression. After the premixed combustion completes, the vessel contents cool and are kept well mixed and at a uniform temperature in the core region using an internal fan [11].

The objective of this study is to analyze the LFL and flame speeds of these lean-dilute fuel-oxidizer mixtures for use in thermodynamic state generation in the CV. The analysis includes determining the flame speed as a function of fuel mixture ($C_2H_2-H_2$) and fuel- O_2-N_2 mixtures.

2. Constant Volume Combustion Vessel

The Michigan Technological University combustion vessel (CV) is similar in design and operation to the CV used in diesel combustion studies at Sandia National Laboratories [11-13]. A photograph of the combustion vessel with the mixing gas panel is shown in Fig. 1 with operating limits shown in Fig. 2.

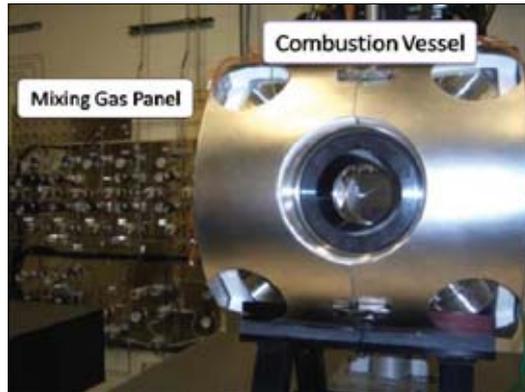


Fig. 1. CV and mixing gas panel

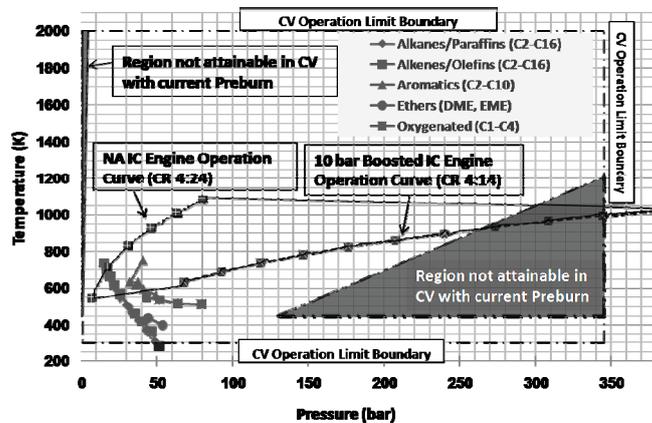


Fig. 2. CV limits with engine curves and fuel critical points

The CV and gas delivery valves are composed of stainless steel, with sapphire windows and steel alloy instrument window fixtures. The combustion chamber is cubical in shape, measuring 101.6 mm on a side and is 1.114 L in volume. In each vertex of the cube is a port that may either house gas intake or exhaust valves, thermocouples, pressure transducers or other instrumentation. Six window ports make up the faces of the cubical chamber. Typically, one window port is used for a fuel injector fixture, one is used for a spark electrode/mixing fan fixture, while the other four hold sapphire windows. These windows allow optical access to the CV for high speed imaging and laser diagnostics of fuel spray, autoignition, and combustion phenomena. The gaseous composition in the vessel can be controlled to match a wide range of combustion chamber environments in modern diesel engines with simulated boost pressure capability to 10 bar. The operation limits for the CV can be seen in Fig. 2 in comparison to diesel engine operation curves, and critical points for a number of fuels.

3. Thermodynamic State Generation

The process in the CV to generate the thermodynamic state and diesel combustion is shown in Fig. 3 with operating limits shown in Fig. 2. The generation of the thermodynamic chamber conditions is accomplished by utilizing a premixed combustion process that is initialized by a spark-ignited burn of a gaseous mixture [11-13]. Gas concentrations in the reactants for the premixed combustion (herein referred to as the “preburn”) are obtained by using a partial pressure fill technique in a separate 10 L high pressure mixing vessel. The mixture is then metered into the CV to fill to the desired density. This mixture is ignited by a spark discharge. In the case shown in Fig. 3 at a density of 14.8 kg/m^3 , the chamber reaches a peak pressure of 7 MPa and temperature of 1850 K. The burned gases then cool due to heat transfer to the vessel walls and windows reducing the chamber pressure and temperature.

During the cool down, when the desired pressure/temperature state is reached, the diesel fuel is injected and if conditions are sufficient, autoignition and combustion of the diesel spray occurs, which is shown in Fig. 3, with the preburn (labeled Premixed Combustion in the figure) being responsible for the initial pressure rise, and diesel injection and autoignition responsible for the smaller pressure rise at $t=0.92$ seconds. The preburn procedure to generate the desired chamber environment has been used extensively in studies of diesel combustion by Naber et al. [11] and Pickett [12]. Naber presented a preburn combustion reaction of H_2 , C_2H_2 , O_2 , and N_2 that was used to generate the environment for diesel injection and combustion. The chemical reaction equation that was used in the preburn is given in Eq. (1) [11].

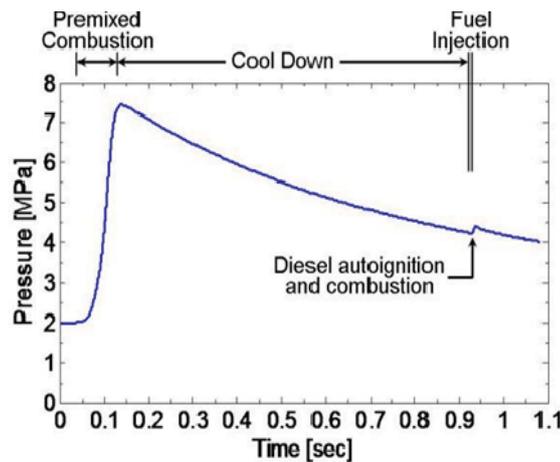


Fig. 3. CV state generation pressure curve for core conditions of 1000 K and 14.8 kg/m^3 [12]

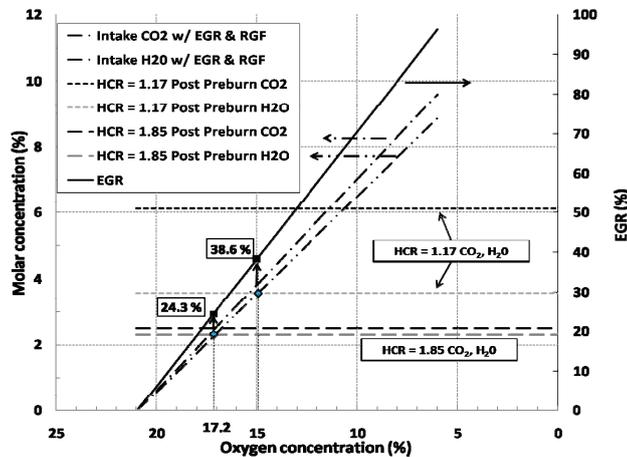
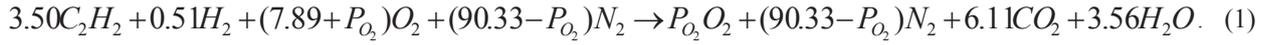


Fig. 4. Intake CO_2 & H_2O comparison: CV vs. Diesel Engine with EGR



In Eq. (1), P_{O_2} in the products is the mole fraction of oxygen, as the equation has been normalized for 100 total moles of products. This combination of combustible gases was chosen to limit water and maximum temperature reached during the preburn combustion, while maintaining robust combustion. The oxygen concentration in the reactants can be varied to control the resulting residual oxygen in the products, P_{O_2} , which is the oxygen content in the gaseous mixture for the main diesel fuel injection. The molar percentage of carbon dioxide and water vapor in the products is 6.11 and 3.56 percent, respectively while the hydrogen-to-carbon ratio (HCR) is 1.17. These levels of CO_2 and H_2O are equivalent to a 38.6 percent EGR (by mass). However, the typical HCR for light diesel fuel is 1.85 [6]. An improvement to the preburn combustion given in Eq. (1) would be to match the HCR of the products of the preburn to that of the diesel fuel.

Shown in Eq. (2) is a preburn combustion equation matching diesel fuel HCR of 1.85. Eq. (2) has again been normalized to produce 100 moles of products. This combustion equation was calculated at the lower flammability limit of the $HCR_{1.85}$ fuel-oxidizer mixture.



The oxygen concentration in the products of Eq. (2) is still controllable for tests simulating EGR rates, including a zero-percent oxygen condition for the study of vaporizing fuel sprays [11] by reducing the reactant oxygen and increasing the nitrogen.

4. Preburn Fuel Fraction Determination and Flame Speed Analysis

A parametric analysis to determine the fuel volume fractions for the preburn charge mixture was performed. This was done to obtain the atomic coefficients for a balanced combustion equation containing C_2H_2 , H_2 , O_2 , and N_2 . Once the atomic coefficients were obtained, the mole fraction of each reactant species was calculated and used as the input reactant fractions in an analysis of laminar flame speed (LFS) using detailed chemical kinetics code [9].

Constraints used in the parametric analysis were conservation of atoms, non-negative atomic coefficients, constant oxygen molar fraction of 21 percent in the products (matching oxygen concentration in atmospheric air), as well as maintaining fuel volume fractions above the lower flammability limit of the fuel mixture (LFL_{mix}), as determined by Eq. (3) [10].

$$LFL_{mix} = \frac{1}{\sum_{i=1}^N \frac{X_i}{LFL_i}} = \frac{1}{\frac{X_{C_2H_2}}{LFL_{C_2H_2}} + \frac{X_{H_2}}{LFL_{H_2}}}. \quad (3)$$

Using this constraint of LFL_{mix} allows for the proper mole fraction of fuel to be returned that could be used for LFS analysis.

The analysis program used for generating Eq. (2) allows for setting of the HCR, making it a valuable tool for analysis of different fuels as well as fuel concentrations in fuel mixtures. The HCR is achieved by varying the molar ratios of H_2 and C_2H_2 in the reactants, while setting the oxygen concentration in the products to the desired value. When this is done, the void created by lowering the oxygen concentration is replaced with nitrogen. Fig. 4 shows the relationship of diesel engine EGR plus residual gas fraction (RGF) in comparison to the original preburn combustion equation (Eq. (1)) and the revised HCR control preburn combustion equation (Eq. (2)), for preburn product oxygen concentrations ranging from 21 percent to 6 percent. The intake CO_2 and H_2O curves show the mole fraction of each constituent that would be in the cylinder gas charge in an operating diesel. The horizontal dashed lines show the mole fraction of CO_2 and H_2O

in the products of Eq. (1) and Eq. (2). The point on the x-axis where the horizontal lines cross the intake $\text{CO}_2/\text{H}_2\text{O}$ lines is the oxygen concentration value in the products of Eq. (1) and Eq. (2). This oxygen concentration corresponds to the equivalent EGR rate that would be simulated in the CV using Eq. (1) or Eq. (2) for state generation. The minimum EGR that can be simulated is 24.3 percent (RGF was one percent by mass) using a post-preburn oxygen concentration of 17.2 percent with matching CO_2 and H_2O concentrations. Oxygen concentration of 21 percent can also be simulated; the mole fraction of the products of the preburn would still, however, contain the mole fractions of CO_2 and H_2O as given in Eq. (2) ($\text{HCR}_{1.85}$) and shown in Fig. 4.

Operating preburn combustion processes near the LFL (lean limit) of the C_2H_2 - H_2 mixture is important to the CV studies. The peak temperature during the preburn is controlled by the mass and respective chemical energy of the C_2H_2 - H_2 fuel charge that is able to react with the oxygen supply. Therefore, using a small fuel mass limits the peak temperatures, and thus pressures, so as not to exceed the operational limits of the combustion vessel (350 bar). Also, for temperatures seen in the CV, related simulation analysis has shown NO values of 28 ppm with a peak CV gas temperature of 1787 K, and 6 ppm with a gas temperature of 1710 K. The reduction of NO in the preburn products is also a benefit of lower combustion temperatures.

Secondly, maintaining a small fuel mass in the preburn assures low concentrations of CO_2 and H_2O in the oxidizer charge mass for the diesel fuel combustion due to low concentrations of H_2 and C_2H_2 in the preburn reactant mixture. Low CO_2 and H_2O is representative of a lower EGR rate. The excess C_2H_2 used in Eq. (1) accounts for the high CO_2 concentration in the preburn products, and thus the high simulated EGR rate. Decreasing the volume fraction of C_2H_2 in the preburn while maintaining a HCR to minimize the CO_2 in the diesel combustion reactants effectively mimics lower EGR rates. Also, when decreasing the fraction of H_2 fuel, the water vapor is reduced, decreasing the vapor pressure and possible condensation in the premixed combustion products during cool down.

Being able to target low EGR rates by preburning at the lean limit of the C_2H_2 - H_2 fuel mixture also gives the flexibility to imitate a wide range of EGR rates. The amount of C_2H_2 in the preburn can be increased which would raise the volume fraction of CO_2 and H_2O in the diesel reactants, simulating higher EGR. With current engine technology and research, the ability to replicate a wide range of EGR rates is a valuable tool in analyzing the effects of the EGR on diesel fuel sprays, and the subsequent ignition and combustion.

5. Laminar Flame Speed

CHEMKINTM software utilizing the PREMIX combustion code was used as a base for the fuel mixture laminar flame speed simulations [9]. Thermal diffusion (Soret effect) was considered with multicomponent transport since H_2 was a main fuel constituent, and both parameters are important in H_2 combustion [14]. The laminar flame speed simulations discussed in this paper assume constant pressure combustion, with the temperature rise associated with the release of chemical energy during the combustion process.

The chemical kinetic mechanism used for all the simulations is the GRI-Mech 3.0 mechanism [1], due to its encompassing abilities of the simulated species. Also, the fuels and products stayed below the mechanisms limit for use with H_2 and C_3 and lower hydrocarbon fuels.

6. State Generation Relation

Flame speed simulations were chosen for analysis of mixtures at the lean and dilute limit because a robust flame will ensure full oxidation of the preburn reactants, as well as stable flame propagation through the mixture, eliminating the possibility of preburn fuels in the reaction products. These reasons led to the conclusion that if the flame does not propagate, required

temperature and pressure will not be reached, and C_2H_2 and H_2 may not be fully combusted.

The platform created through EES [3] and CHEMKINTM to determine preburn fuel-oxidizer mixtures that achieve stable combustion with proper product molar fractions will be a valuable tool for ongoing experiments. The preburn fuel-oxidizer mixtures were calculated based upon concerns for providing a gaseous environment that is representative of the combustion chamber in an operating diesel engine, while minimizing the simulated EGR rate within the combustion vessel prior to diesel fuel injection. Data values will be obtained that give the minimum H_2O and CO_2 and resulting EGR rate floor, with higher rates of EGR also enabled.

The reaction flowchart for a complete CV cycle is shown in Fig. 5. The flowchart shows how the preburn products are tied to the diesel combustion oxidizer charge.

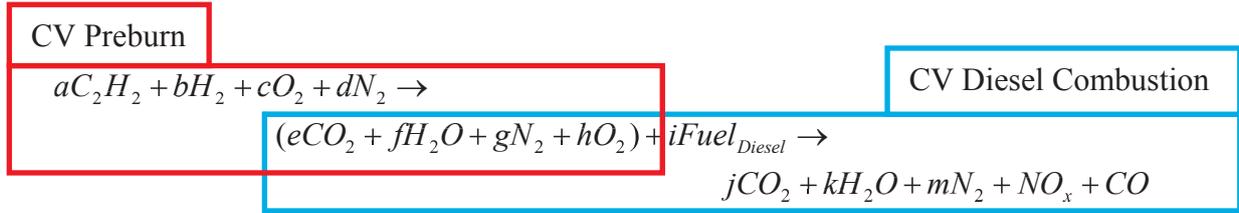


Fig. 5. CV Preburn to diesel combustion chemical flowchart

Seeing this relationship is important for understanding that accurate and optimal state generation depends on correct preburn reactant mixtures to be used in the combustion vessel. Reactant coefficients (a, b, c and d) are controllable, so it is possible to obtain a wide range of mixtures of these species. Further explanation of the procedure to control gaseous concentrations is located in the Results and Discussion section. It must be considered though that the reactants and products in Fig. 5 show the case of ideal combustion and that minor species including NO also exist in the products.

The results obtained from the simulations presented in the current study will be verified by further combustion simulations for a constant volume combustion vessel, as well as validated experimentally in the laboratory. The further simulations will confirm whether or not the fuel-oxidizer mixtures used in the flame speed calculations will reach the required pressures and temperatures for diesel fuel injection and combustion while including heat transfer effects during the cool down of the combustion vessel. Both sets of simulation data will give insight into predictions of experimental tests that will later be conducted in the CV laboratory.

7. Results and Discussion

Initial conditions for simulations were set at a pressure of 1 atm and a temperature of 450 K. The pressure was chosen as a base pressure while the temperature was 450 K, which is the temperature of the CV walls and gases of CV prior to spark ignition [11]. A near linear relation is observed in the flame speed. The mixture air-fuel-ratio, AFR_{mix} , was calculated as the mass of the N_2 - O_2 mixture divided by the mass of the fuel. The stoichiometric AFR, AFR_{stoich} , was calculated as the mass of the stoichiometric (for the actual fuel mass) N_2 - O_2 mixture divided by the actual mass of the fuel. The relation can be seen in Eq. (4) where q is the stoichiometric air multiplier for a C_xH_y fuel, in this case $x = 2$ and $y = 4$ for C_2H_2 - H_2 mixtures and β is the molar ratio of N_2 to O_2 . The equivalence ratio, Φ , is defined as AFR_{mix} divided by AFR_{stoich} .

$$AFR_{mix} = \frac{m_{N_2+O_2}}{m_{C_2H_2+H_2}} \quad AFR_{stoich} = \frac{q(MW_{O_2} + \beta MW_{N_2})}{m_{C_2H_2+H_2}} \quad \text{where } q = \frac{5N_{C_2H_2} + N_{H_2}}{2} \quad \text{and } \beta = \frac{N_{N_2}}{N_{O_2}}. \quad (4)$$

Fig. 6 shows the plot of flame speed and combustion temperature for the four fuel mixtures.

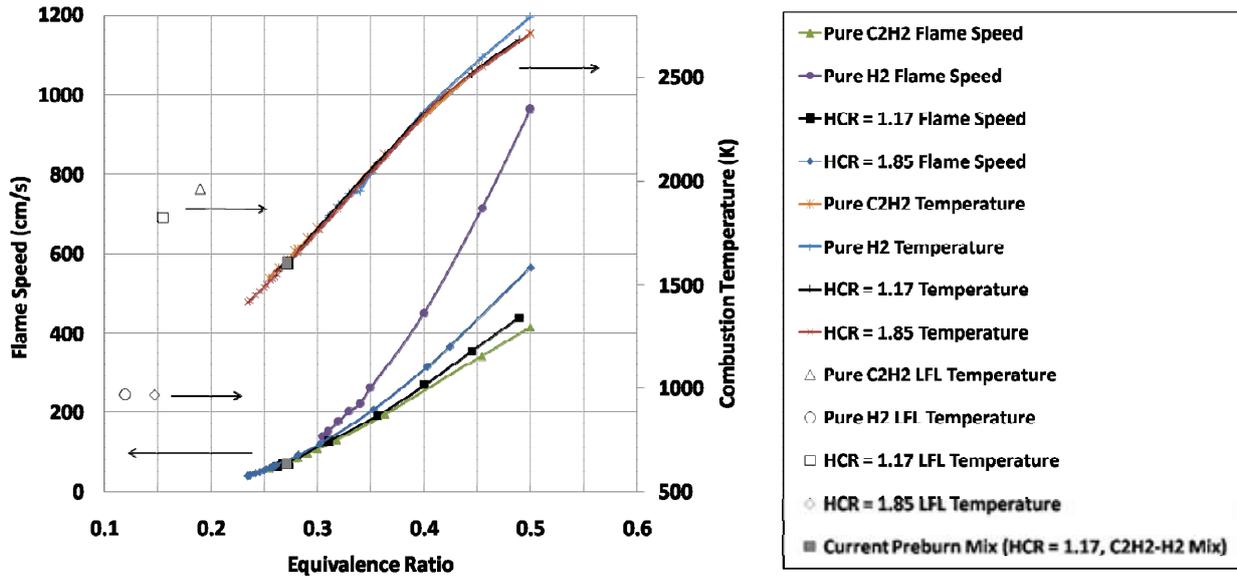


Fig. 6. Combined flame speed and temperature plot for preburn mixtures with 21 percent O_2 in the products

In Fig. 6 the preburn product oxygen concentration is held constant at 21 percent and the equivalence ratio is varied from 0.50 to the lean limit by reducing the moles of fuel in proportion to the oxygen. The current fuel mixture is shown on Fig. 6 alongside other fuel mixtures, comparing the combustion temperature and flame speed to simulated mixtures.

The generation of the state in the CV depends on the composition of the input gases, and can be modified as desired for varying conditions of EGR rate, residual mass fraction, and oxygen concentration. The main concern with the generation of the state after the preburn is that the temperature and pressure, oxygen concentration, and HCR of the CO_2 / H_2O gas mixture represent an operating engine. Sufficient temperatures and pressures must be created to match compression temperatures, hence even though there are leaner mixtures than the current mixture, the use of one of these mixtures may not suit the requirements of the successive diesel combustion tests.

Fig. 7 shows the relation of flame speed to combustion temperature as the mixtures approach the lean limit fuel. The dashed horizontal line in the plot is the flame speed generated using the current mixture (the point marked by the black rimmed dot at a temperature of 1600 K).

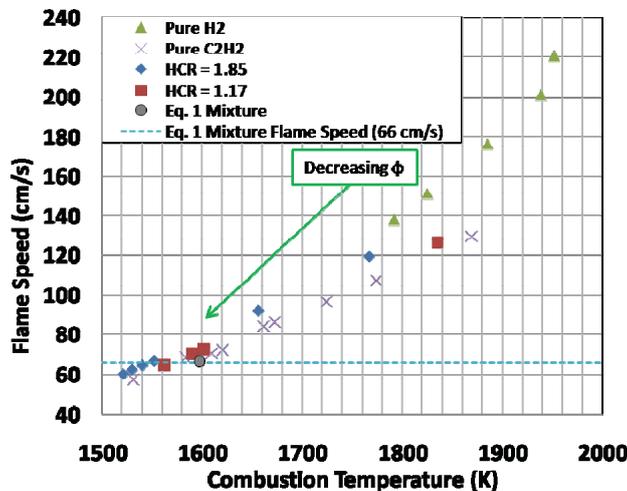


Fig. 7. Flame speed versus combustion temperatures for decreasing equivalence ratios from 0.50 to the lean limit for 21 percent O_2 premixed combustion products

Tab. 1 shows the comparison between all fuel cases with respect to reactant fuel mole concentration, HCR, flame speed, temperature, and product concentrations, all for simulated cases of flame speed equal to approximately 66 cm/s with a post reaction concentration of 21 percent O₂. Between the HCR_{1.17} and HCR_{1.85} equations, the HCR_{1.85} equation has a slightly lower CO₂ concentration and slightly higher H₂O concentration, which would be expected as the ratio of the H₂ to carbon is higher in this mix. A benefit is that the HCR_{1.85} equation still maintains the HCR of diesel fuel, while the HCR_{1.17} equation does not. Using the point from the HCR_{1.85} equation that corresponds to a similar flame speed as the HCR_{1.17} equation (seen in Tab. 1 in the S_L column of the HCR_{1.85} row), oxygen sweeps were done to generate Fig. 8 and Fig. 9.

Tab. 1. Fuel Mixture Comparison

Fuel Mix	HCR	X _{H₂,R}	X _{C₂H₂,R}	X _{O₂,P}	Y _{CO₂,P}	Y _{H₂O,P}	S _L (cm/s)	T (K)	Avg. Premixed Combustion Duration (ms)	0-10% Mass Fraction Burned Duration (ms)	10-90% Mass Fraction Burned Duration (ms)
H ₂	NA	0.155	0.000	0.210	0.000	0.112	69	1587	NA	NA	NA
C ₂ H ₂	1.00	0.000	0.032	0.210	0.095	0.019	68	1621	NA	NA	NA
HCR _{1.17}	1.17	0.005	0.030	0.206	0.091	0.022	66	1597	64.1	15.2	34.6
HCR _{1.85}	1.85	0.022	0.026	0.207	0.080	0.030	66	1572	52.7	8.3	30.3

The calculated mass fraction burned (MFB) in the HCR_{1.85} equation is faster than the HCR_{1.17} equation due to the increased H₂ content. This trait is also reflected in the premixed combustion duration shown in Tab. 1 by the reduced combustion duration of the HCR_{1.85} mixture at 52.73 milliseconds (ms), to 64.10 ms of the HCR_{1.17} mixture, a difference of approximately 11.4 ms.

Using the HCR_{1.17} (Eq. (1)) and HCR_{1.85} (Eq. (2)) equations, a sweep of preburn reactant oxygen concentration was performed to produce the data shown in Fig. 8 (post preburn oxygen concentrations from 21 to 0 molar percent). Throughout the oxygen sweep, fuel mole fraction was kept constant at 3.50 percent for the HCR_{1.17} equation and 4.79 percent for the HCR_{1.85} equation by replacing reduced oxygen with excess nitrogen, effectively forcing the reaction from a fuel lean reaction to a stoichiometric reaction with high nitrogen dilution. The starting point at an oxygen concentration of 21 percent was chosen by matching the flame speed of the HCR_{1.85} mixture with the current flame speed of the HCR_{1.17} mixture.

Fig. 9 shows the relation of flame speed to combustion temperature for the HCR_{1.17} and HCR_{1.85} mixtures as the reaction products approach 0 percent oxygen (starting from 21 percent oxygen and reducing the oxygen concentration). This plot also shows the relation of reduced flame speed and increased combustion temperature as the equivalence ratio increases.

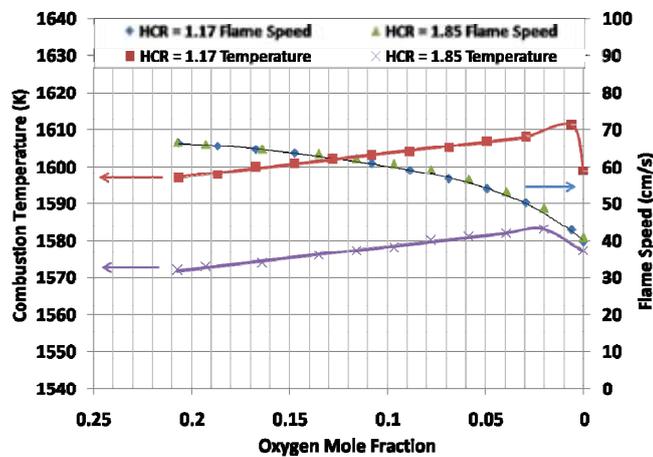


Fig. 8. Combustion temperature and flame speed for HCR fuel mixtures with constant fuel mole fraction with decreasing post-combustion oxygen concentration (approaching stoichiometric combustion)

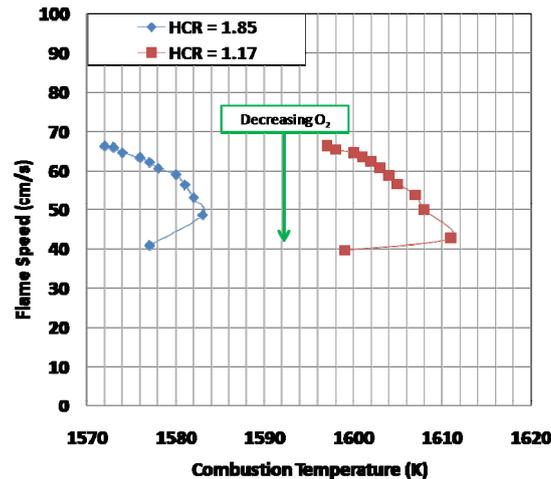


Fig. 9. Flame speed vs. combustion temperature for HCR fuel mixtures with constant fuel mole fraction with decreasing post-combustion oxygen concentration (approaching stoichiometric combustion)

The increasing combustion temperature can be attributed to the lower specific heat of the nitrogen [15] that replaces the oxygen in the mixture as the oxygen concentration in the reaction is reduced. The reduced flame speed can be attributed to the increased dilution from the increased nitrogen [8]. Temperatures in the sweep rose from a minimum of 1597 K and 1572 K (for the HCR_{1.17} and HCR_{1.85} mixes, respectively) to maximums of 1611 K and 1583 K, respectively while flame speeds dropped from 66 cm/s to 39 cm/s (HCR_{1.17}), and 66 cm/s to 40 cm/s (HCR_{1.85}).

8. Summary and Conclusions

The premixed burn mixtures of H₂-C₂H₂ fuels were investigated using CHEMKINTM to identify the fuel fraction values of the H₂ and C₂H₂ that could be used for thermodynamic state generation in a constant volume combustion vessel with a target fuel HCR of 1.85 matching that of diesel fuel. Simulations were completed under constant pressure combustion conditions with an initial temperature of 450 K. The basis for the simulations included the objective to minimize the simulated EGR rate by the reduction of CO₂ and H₂O and matching the hydrogen to carbon ratio in the preburn combustion products. Minimizing the EGR will show the lowest level that can be achieved while maintaining a complete combustion in the CV, with the higher EGR rates easily obtained by increasing the fuel concentrations.

For the HCR_{1.85} mixture, combustion temperatures are lower for similar flame speed conditions. Flame speeds were similar between the two mixtures for each post-combustion oxygen concentration even though the H₂ molar concentration in the HCR_{1.85} is higher. The combustion duration of the HCR_{1.85} mixture was shorter than the HCR_{1.17} mixture. When comparing the CO₂ and H₂O emissions combined, the calculated mass of these two species (in relation to the mass of all combustion products) totals 11 percent by mass for both mixtures (see Tab. 1 Y_{CO2} and Y_{H2O}).

For the case of the HCR_{1.85} mixture, the higher concentration of H₂ in the fuel mix extends the lean limit of the fuel mixture to a lower equivalence ratio ($\Phi=0.147$) than that of the HCR_{1.17} mixture ($\Phi=0.156$) as seen in Fig. 6. Also, for the HCR_{1.85} fuel mixture, lower temperature premixed combustion events can be utilized, lowering the NO_x formation during the preburn.

Additional investigations could cover separate chemical kinetic mechanisms for the diesel autoignition to assess the impact of the preburn on the diesel combustion process. Fuel mixtures of CO, C₂H₄ and other gases should also be studied for flame speed, temperature and residual compositions. Fuel mole fraction reduction can be investigated to find the stable combustion limit for the premixed burn, as this would reduce the amount of CO₂ and H₂O in the premixed combustion products (reducing the EGR floor). These simulations were conducted at 1 atm while

the vessel can operate up to 350 atm, therefore, pressure effects on flame speed and combustion temperature should be investigated for the fuel mixtures presented in this work.

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