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Ignition, Flame Propagation, and End-Gas Autoignition Studies of Natural Gas/EGR Blends in a Rapid Compression Machine

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Abstract: The development of high efficiency, spark ignited natural gas engines is currently limited by engine knock at high power density (at high compression ratio and/or elevated boost pressures) and misfire (at lean conditions and/or high exhaust gas recirculation levels). The knock and misfire limits are further confounded by the wide variety in fuel reactivity observed in "pipeline quality" natural gas. In this study, a rapid compression machine (RCM) was used to characterize the effects of variation in natural gas fuel reactivity and exhaust gas recirculation (EGR) on homogeneous ignition delay, flame propagation rate and end-gas autoignition (EGAI) propensity for stoichiometric natural gas/oxidizer/EGR blends. Pipeline quality natural gas with variable reactivity (68 < Methane Number < 95) was simulated using mixtures of methane, ethane, and propane. EGR was simulated with mixtures of Ar, CO_2, CO, and NO. EGR substitution rates were varied from 0 to 30 mass percent. Ignition delay period under homogeneous autoignition conditions was measured at compressed pressures of 24.0 to 33.1 bar and compressed temperatures of 667 to 980 K. Flame propagation rate and EGAI propensity was measured at spark-ignition pressures of 29.9 to 32.9 bar and temperatures of 721 to 782 K.

Keywords: Ignition Delay, Flame Propagation Rate, Rapid Compression Machine, Methane Number

1. Introduction

Spark-ignited (SI), natural gas (NG), engines offer a multitude of advantages over diesel engines including lower particle emissions and lower cost (engine maintenance, exhaust treatment systems, and fuel) [1]. However, limited fueling infrastructure and wide regional variances of fuel reactivity make high performance, high boost SI-NG engines difficult to develop. Currently, SI-NG engines need to be able to run on the highest reactivity (lowest quality) fuel and are unable to take advantage of higher quality fuel if available. In order to maximize performance and efficiency, mobile NG engines will need to be able to run on the threshold of knock. To accomplish this SI-NG engines will need to be able to utilize the fuel reactivity across any region. Such engines will likely require high percentage of exhaust gas recirculation (EGR) and stoichiometric air/fuel ratios to maintain transient load performance. The purpose of this study is to investigate the effect of NG fuel reactivity and EGR substitution on homogenous ignition delay, flame speed, and fractional end-gas autoignition (F-egai) of NG blends using a rapid compression machine (RCM). The results of this study will be used to inform future chemical kinetic model reduction and development.

In the United States the majority of NG is made up of light alkane fuels. In a study done by the Southwest Research Institute in 2014 [2] regional compositions were measured and averaged. The

abbreviated results of that study and the measured natural gas composition at the Colorado State University (CSU) Powerhouse Campus are outlined in Table 1 below.

Table 1: Regional average of "pipeline quality" natural gas mixtures in the United States [2] and measured at Colorado State University Powerhouse Campus. (% mole fraction)

Region	Methane	Ethane	Propane	Nitrogen	Carbon dioxide	Other
Western	94.6%	3.2%	0.5%	0.8%	0.8%	0.2%
Central	94.7%	3.5%	0.3%	0.9%	0.6%	0.1%
Eastern	92.7%	4.1%	0.4%	0.9%	1.7%	0.2%
Colorado State University	85.5%	8.9%	1.2%	1.0%	1.6%	1.9%

The majority of NG composition in the United States is, methane, followed by ethane and propane (C1-C3) with trace amounts of butane and other containments including nitrogen, hydrogen, carbon dioxide, etc. In Table 1 the regional averages have mild variances in composition. However, if the composition measured at CSU is compared to the western regional average there is a large variance in fuel quality. In order for mobile NG SI engines to be effective they need to be able to accommodate these large variations in fuel quality from any source. Since mobile NG engines would be refueled at specific fueling stations not the regional average. Therefore, the fuels used in this study span 68-95 methane number using blends of C1-C3. The problem of fuel reactivity is complicated further with the addition of EGR. Historically, EGR has been used in engines to reduce nitric oxide (NO_x) formation and has been shown to prevent knock in SI engines [3]. The majority of these studies use nitrogen as an EGR surrogate for simplicity. However, EGR composition varies greatly from engine to engine, if the EGR is taken pre/post catalyst, is wet/dry, hot/cooled, etc. The majority of EGR composition is nitrogen, carbon dioxide, and water vapor with trace amounts of nitric oxides, carbon monoxide, and unburned fuel. This study attempts to better understand the knocking tendencies of varied reactivity C1-C3 fuel blends with a more detailed EGR surrogate.

2. Methods / Experimental

The CSU RCM (figure 1) lends itself well to homogenous ignition delay, flame speed, and EGAI measurements due to its horizontally opposed dual piston construction (symmetrical compression) and optical access. The RCM was set up in two configurations for two sets of experiments.

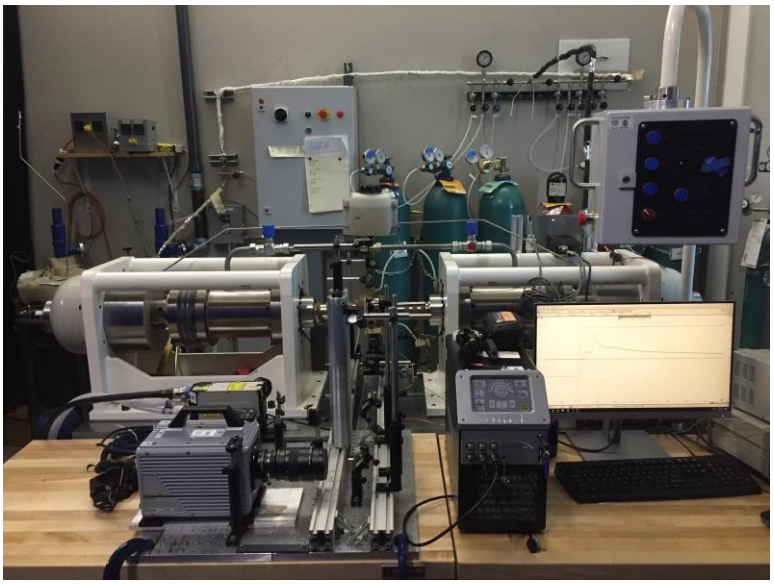

Figure 1: Colorado State University rapid compression machine. The CSU RCM uses dual horizontally opposed pistons to maintain symmetrical compression. The above configuration uses an Nd:YAG laser as the ignition system and uses schlieren imaging to observe flame propagation rates

2.1 CSU RCM Configuration to Measure Homogenous Autoignition Delay

Homogenous ignition delay experiments utilize creviced pistons to reduce roll-up vortices. Minimizing roll up vortices reduces intrusion of the cold wall thermal boundary into the adiabatic core of the chamber. Combustion is induced by the heat and pressure generated from the compression of the RCM pistons. A high speed pressure transducer (Kistler 601CAA) measures the pressure inside the combustion chamber during a combustion event. The temperature inside the combustion chamber is estimated using ideal gas law and adiabatic compression assumption from the measured pressures. The homogenous ignition delay is defined as the time between the compressed pressure at top dead center (TDC) and the maximum pressure rise rate (first derivative) during the combustion event.

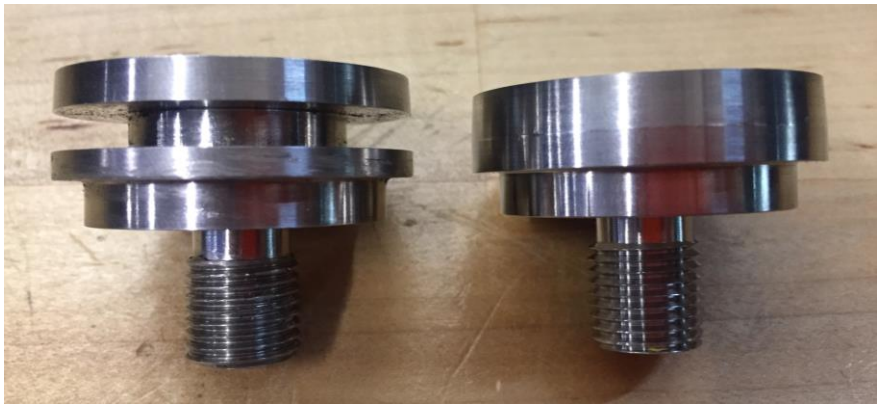

Figure 2: Left: Photo of creviced RCM piston used in homogenous ignition delay experiments Right: non-creviced pistons used for flame speed and F-egai experiments.

2.2 CSU RCM Configuration to Measure Flame Propagation Rate and Fractional End-Gas Autoignition

In order to measure flame propagation and F-egai, a laser ignition system and optical schlieren system was developed for the RCM. The laser ignition system consists of a pulse-delay generator controlled 1064nm Nd:YAG laser. The beam from this laser is steered through a beam splitter that directs a small portion of the beam to a photodiode to get laser timing. Another beam splitter directs another small portion of the remaining beam to an energy meter to get a relative spark energy. The remaining portion of the beam is then steered to the combustion chamber where a lens focuses the energy down to a point in the center of the combustion chamber creating a spark. The schlieren system uses a bright LED and a series of optics to pass collimated light through the chamber. The collimated light is refracted in the chamber by density gradients (high temperature/density change at the flame front) and the light is then collected by a high speed camera (50,000 FPS) allowing optical measurements inside the combustion chamber of the RCM. See figure 3 below for a detailed diagram of the systems used in the CSU RCM.

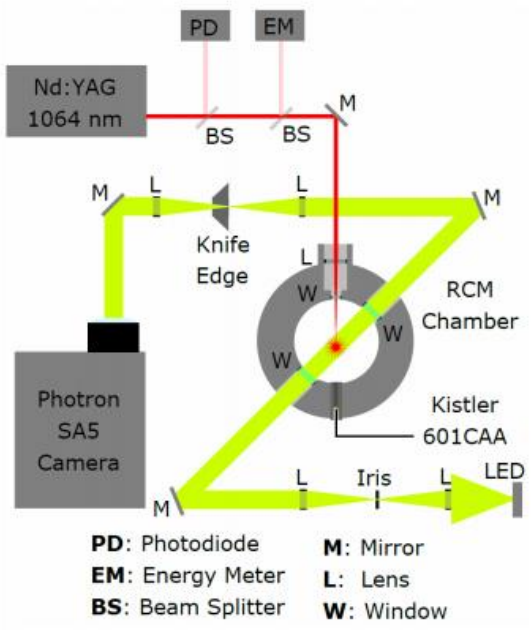

Figure 3: Schematic of CSU RCM laser ignition and schlieren system [4].

In order to be able to separate the flame propagation from the end-gas autoignition event all of the combustion must be in the main combustion chamber. With the creviced pistons there is potential for ignition to occur in the crevice volume that may or may not be end-gas autoignition. It is also difficult to distinguish this by looking at the apparent heat release rate (AHHR) of the combustion event. Therefore non-creviced pistons were used for the flame propagation and F-egai experiments (figure 2). In these experiments the initial conditions are designed to have a mixture that does not ignite under compression. The ignition source is the laser spark that is injected into chamber about 10 ms after compression. The spark ignites the mixture and a spherical flame propagates outward through the chamber. As the spherical flame propagates outward the end-gas is heated and compressed eventually igniting. This ignition is EGAI conventionally called knock in engines.

2.3 Flame Propagation Measurement

Flame propagation rate is measured using the schlieren images collected from the RCM. Flame radius vs time was measured from the images. However, due to the spherical nature of these flames, there is a flame stretch associated with the flame propagation. In order to correct for this methods using the non-linear extrapolation correction developed by Kelly and Law [5, 6].

$$s_b = s_b^0 t + cr_f + 2L_b \ln(r_f) - 4\frac{{L_b}^2}{r_f} - \frac{8}{3}\frac{{L_b}^3}{r_f} \quad (1)$$

Where s_b is the burned propagation rate approximated with a second-order polynomial in cm/s, s_b^0 is the zerostretch burned propagation rate to be found in cm/s, t is time in s, c is a measurement constant, r_f is the equivalent spherical flame radius in cm, and L_b is the Markstein length in cm.

The extrapolated zero-stretch burned propagation rate was then converted to an unburned propagation rate by using equation Eq. (2) [6].

$$s_u = s_b \left(\frac{\rho_b}{\rho_u}\right) \quad (2)$$

Where *s* is the flame propagation rate in cm/s, ρ is the region density in kg/m3, and the *u* and *b* subscripts represent the unburned and burned regions across the flame respectively. Unburned density is calculated using the initial pressure and known compression ratio. Burned density was approximated using adiabatic flame temperature calculated using GasEq.

2.4 Fractional End-Gas Autoignition Description

Fractional ends-gas autoignition (F-egai) is the fractional percentage of the heat released during the combustion that is attributed to volumetric end-gas autoignition with respect to the net total amount of heat release during the entire combustion event. This is done by utilizing the apparent AHHR history of the combustion event. The AHRR is calculated using the constant volume process.

$$AHRR = \frac{dQ}{dt} = \frac{1}{\gamma - 1} V \frac{dP}{dt} \quad (3)$$

Where *V* is the gas volume after compression in m^3, γ the ratio of specific heats of the mixture, *P* the pressure in Pa and *t* the time in s.

F-egai is then calculated as follows:

$$f_{EGAI} = \left[\int \frac{dQ}{dt}\, dt\right]_{EGAI} / \left[\int \frac{dQ}{dt}\, dt\right]_{total} \quad (4)$$

Where $\frac{dQ}{dt}$ is the apparent heat release rate in W. The numerator is integrated heat release during EGAI in J, and the denominator is the integrated total heat release in J.

A more detailed description of the flame speed calculations and F-egai can be found in reference [4].

2.5 Experimental Mixtures and Test Conditions

In this study, two "pipeline quality" fuel blends were studied which are outlined below in Table 2.

Table 2: Natural gas test blends used in this study. (% mole fraction)

Name	Methane	Ethane	Propane	Methane Number
Dry Blend	99.0%	0.5%	0.5%	95
Wet Blend	82.0%	15.0%	3.0%	68

The two fuel blends were then mixed with a synthetic EGR mixture. The composition of the synthetic EGR mixture used in this study was informed from exhaust composition measurements of a Cummins medium duty SI-NG mobile engine. In order to maintain simplicity, a single synthetic EGR was used for this study. To maintain compatibility with the CSU RCM two changes to the measured EGR compositions were made. The first, is the substitution of carbon dioxide for the water vapor measured in the actual EGR. This is required to ensure good mixing and delivery of the synthetic EGR with the rest of the reactants in the RCM combustion chamber. The carbon dioxide substitution percentage is selected to maintain ratio of specific heats of the entire EGR mixture. The second change is the replacement of nitrogen in the EGR mixture with argon. Argon is required in the CSU RCM to reach a higher compressed pressure and temperature. Therefore, since the inert gas of the reactant mixture was argon the inert gas in the EGR had to be changed to argon. This maintained a similar relative change in ratio of specific heats as what would be seen in an engine running on air with a nitrogen based EGR. Following these two changes the final composition of the synthetic EGR gas is outlined in table 3 below.

Table 3: Synthetic EGR mixture used for

Species	% Mole Fraction
Argon	79.3%
Carbon Dioxide	20.0%
Carbon Monoxide	0.35%
Nitrogen Monoxide	0.35%

The substitution was calculated by mass using the following equation.

$$EGR\% = \frac{mass\_EGR}{(mass\_EGR + mass\_air + mass\_fuel)} \quad (5)$$

Table 4 outlines the eight reactant mixtures in mole fraction.

Table 4: Reactant mixtures used in current study.

Fuel Type	EGR Subs. (Mass %)	Fuel (Mole %)	AR (Mole %)	O2 (Mole %)	EGR (Mole %)
Dry	**0**	0.094	0.716	0.190	0.000
Dry	**10**	0.086	0.722	0.173	0.090
Dry	**20**	0.077	0.729	0.156	0.182
Dry	**30**	0.068	0.736	0.138	0.276
Wet	**0**	0.083	0.724	0.193	0.000
Wet	**10**	0.076	0.730	0.175	0.091
Wet	**20**	0.068	0.737	0.157	0.184
Wet	**30**	0.060	0.743	0.139	0.279

For the homogenous ignition delay experiments, each fuel blend is tested at three different initial temperatures (308, 318, and 328 K) resulting in three different compressed temperatures at similar compressed pressure. Data is selected where the compressed temperature of each run was within +/- 10 K of the average compressed temperature of five replicates.

For the flame speed and F-egai experiments, initial conditions were maintained at 1 bar initial pressure and 298 K initial temperature. Since the majority of the EGR mixture is argon, substitution of EGR into the fuel/"air" mixture has a minimal impact on ratio of specific heats resulting in a similar compressed pressure and temperature. Each test case was replicated ten times and two techniques were used for data selection, one for flame speed, the other for F-egai. For flame speed selection piston offset is used. The CSU RCM has two horizontally opposed pistons. Due to friction and other irreversible properties one piston can hit TDC before the other piston reaches TDC, known as piston offset. This offset results in variable turbulent kinetic energy inside the chamber and dramatically changes the flame propagation rate. Therefore, the flame speed results were taken by averaging the replicates out of a total of ten replicates whose piston offsets are less than 4 ms. For the F-egai cases, the data is selected by averaging the replicates whose temperature at the time of the spark is within +/- 10 K of the average of a total of ten replicates. A table outlining the average pressure and temperature at the time of spark is shown below (Table 5).

Table 5: Average temperature and pressure in RCM chamber at time of spark for F-egai experiments.

Fuel Type	EGR Subs. (Mass %)	Pressure at Spark [bar]	Temperature at Spark [K]
Dry	**0**	31.8	782
Dry	**10**	32.2	755
Dry	**20**	31.9	755
Dry	**30**	30.5	768
Wet	**0**	29.9	721
Wet	**10**	31.8	780
Wet	**20**	32.9	781
Wet	**30**	31.5	759

3. Results and Discussion

3.1 Homogenous Ignition Delay

The results of homogenous ignition delay are shown below in figure 4.

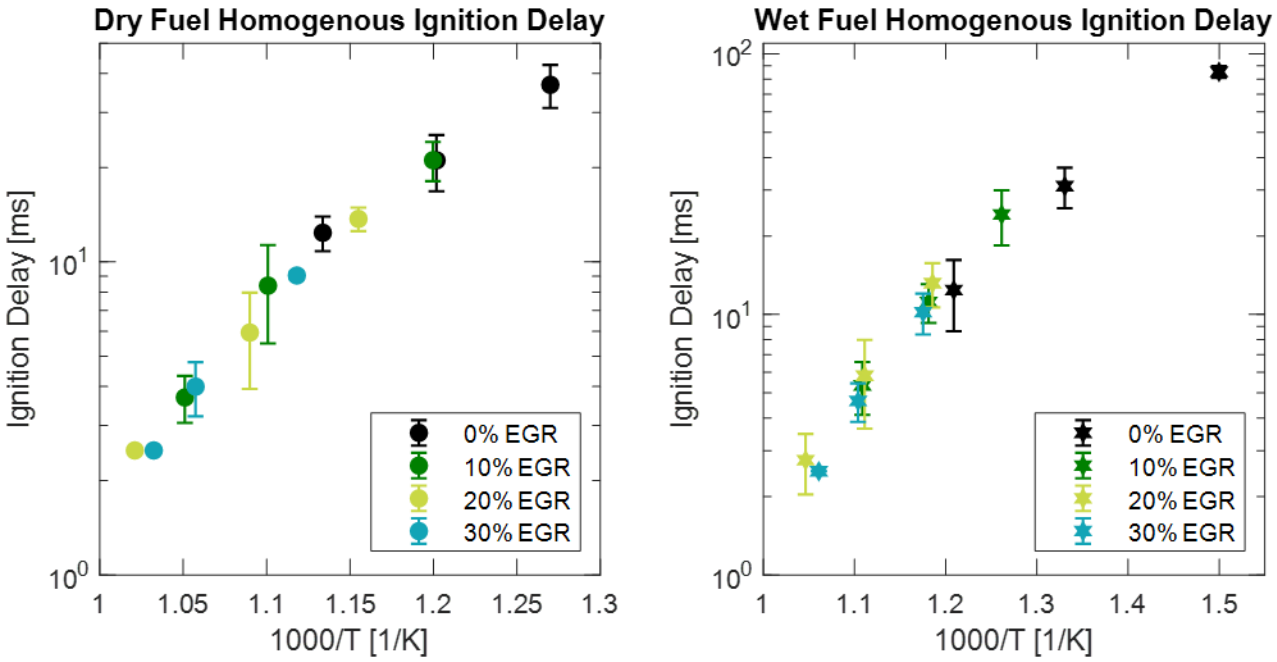

Figure 4: Left: Homogenous ignition delay of dry fuel at 0 - 30% EGR substitution. The average pressure is 31.3 bar with a range from 28.4 – 33.0 bar. Right: Homogenous ignition delay of wet fuel at 0 - 30% EGR substitution. The average pressure is 29.6 bar with a range from 24.0 – 31.9 bar. Error bars are 95% confidence intervals.

The main purpose of these experiments is to see if EGR is causing any chemical kinetic reaction time changes to the two fuel blends. For example, nitrogen monoxide (NO) is a highly reactive species and could potentially impact chemical induction times and knock propensity in engines. These homogenous ignition delay results show linear trends on a log vs. 1000/T plot. This linearity implies that substitution of EGR has very little impact on homogenous ignition delay if the mixtures are at the same temperature. The four points on the wet fuel plot at 1000/T of 1.2 is a good example of this. The ignition delays at that point are all within the error bars at roughly the same temperature. This trend appears at multiple points for both fuel blends. Therefore, the synthetic EGR (dry EGR with high CO/NO concentrations) used in these experiments has very little impact on chemical induction time. In other words, EGR is not making the mixture any more or less susceptible to autoignition (knock) on a chemical kinetic level.

3.2 Flame Speed and F-egai Results

Although the chemical induction time is not affected by EGR substitution flame speed and F-egai are very sensitive EGR substitution rates. The effect of EGR substitution on flame speed and F-egai are shown below in figure 5.

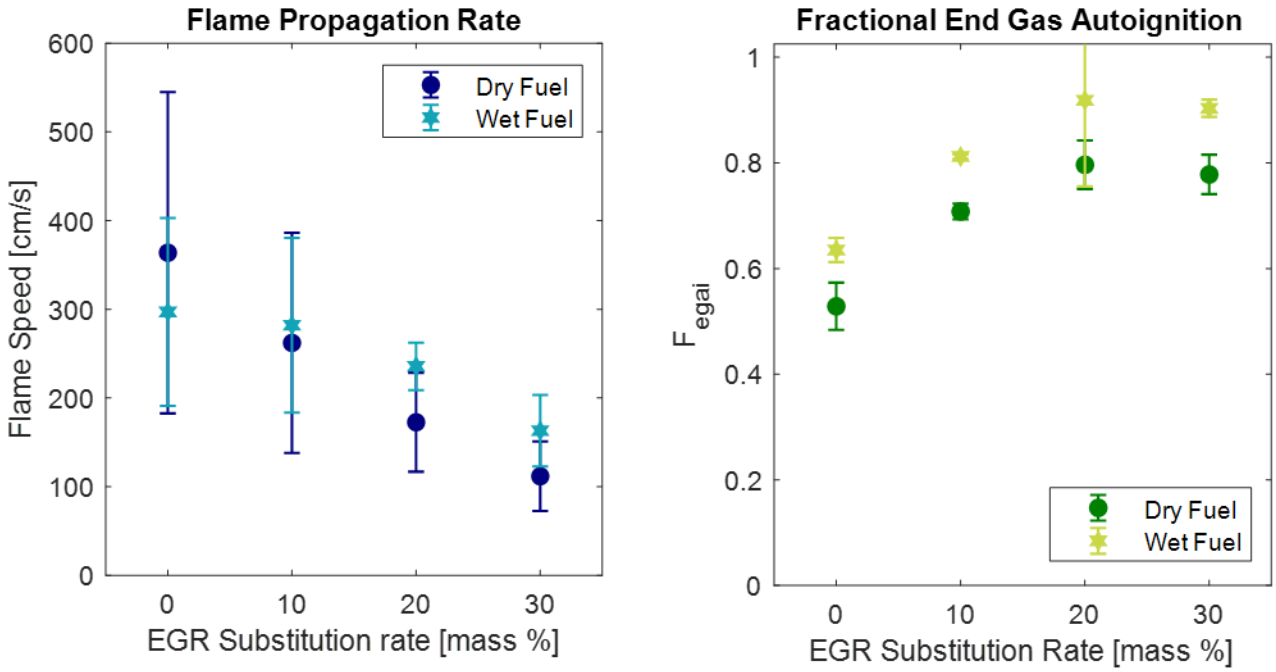

Figure 5: Left: Flame propagation rate at EGR substitution rates 0-30%. Right: Fractional end-gas autoignition (F-egai) at EGR substitution rates 0-30% pressure and temperature at time of spark can be referenced in table 5. Error bars are 95% confidence intervals.

The flame propagation rate in these experiments is not laminar flame speed. With non-creviced pistons the turbulent kinetic energy inside the chamber varies dramatically from test to test resulting in turbulent flame speeds. Since flame speed is so closely related to turbulence the error in these measurements is large (up to 350 cm/s). However, even with the large error, there is a very strong trend between flame speed and EGR substitution rate. The flame propagation rate is dramatically reduced with the addition of EGR substitution. The slower flame speed results in a longer time for the fuel to be consumed. Therefore, the end-gas is heated by the flame for a longer

period of time and there is more time for reactions to occur. Furthermore, there is more end-gas to consume and as a result the F-egai increase with EGR substitution rate. This trend is opposite to what other have seen in engines where EGR substitution decreases knock propensity. However, there are significant differences between a RCM and engine. The CSU RCM completes a compression stroke then locks the pistons at TDC to make a constant volume chamber. Without an expansion stroke the end-gas is not rapidly cooled to slow chemical induction period and cool the reactants temperature. In an RCM the end-gas is heated much longer resulting in a system that is much more likely to knock compared to an engine. EGAI (knock) is a competition between the chemical induction period, the flame heating the end-gas, and the cooling of the expansion stroke. Another note of interest is although EGR substitution causes the flame propagation rate to decrease the two different blends react in different ways. The rate at which the flame speed decreases with the wet fuel is much slower than that of the dry fuel. Indicating that changes in flame speed with EGR substitution are fuel specific. This difference in fuel reactivity is also seen in the F-egai results. Comparable with theory the more reactive fuel autoignites sooner resulting in a larger portion of the end-gas igniting resulting in a larger F-egai. This trend is expected and the rate of change of F-egai with EGR substitution seems to be consistent between the two fuels.

4. Conclusions

The main purpose of this study was to investigate the change that EGR substitution has on pipeline quality NG mixtures from a chemical kinetic standpoint. Homogenous ignition delay seems to remain largely unaffected by the small quantity of NO/CO/CO_2 reactants introduced by EGR. However, flame propagation rate is very sensitive to EGR substitution. As EGR substitution increases the flame speed of the mixture decreases. The rate at which the flame speed decreases is unique to each fuel blend. This indicates that EGR substitution could impact the same engine in different ways if the fuel reactivity changes. This would be important in mobile SI-NG engines. As fuel reactivity increases the F-egai also increases. As EGR substitution increases F-egai also increases due to slower flame speeds consuming less fuel in more time allowing more fuel to be ignited as an end-gas. Future work will expand this study to more fuel blends and help inform chemical kinetic model development at CSU.

5. Acknowledgements

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6. References

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