A Study on the Effect of Ethanol Addition on Laminar Flame Speed of a Four-Component Gasoline Surrogate at Elevated Pressure and Temperature

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1   Introduction

Interest in biofuels has increased recently due to the environmental issues that conventional fuels (i.e., fossil fuels) have. Among these conventional fuels is gasoline. According to the U.S. Energy Information Administration [1], 142 billion gallons of gasoline were consumed by motor vehicles in 2019 in the United States alone. Besides, 197 million gallons of gasoline were consumed in the aviation sector. Therefore, gasoline is a major fuel in the United States. These facts brought the attention of different governmental agencies to the harmful impacts of conventional fuels on the environment. For example, the U.S. Department of Energy has started several initiatives to alleviate any harmful effects to the environment caused by conventional fuels, or any energy-related matters. Among these initiatives is the Co-Optimization of Fuels & Engines (Co-Optima), which aims to investigate, understand, and provide alternatives and solutions for conventional fuels. The Co-Optima initiative has provided ten blendstocks that can serve as alternatives (or additives) to gasoline [2]. Ethanol comes to the top of the list as one of the most promising alternatives for gasoline. Ethanol can also be used as an additive to increase Research Octane Number (RON) and reduce soot emissions [3]. Thus, accurate chemical kinetics mechanisms are vital to the future use of ethanol as a gasoline replacement/additive. This observation led to an increase in work on providing experimental data for ethanol/gasoline fuels to ultimately be used as validation targets for chemical kinetics mechanisms. Laminar flame speed, typically measured experimentally, is an important fundamental parameter that is routinely used to validate kinetic mechanisms of fuels.

For instance, Mannaa et al. [4] developed a new gasoline surrogate and used laminar flame speed and Markstein length as the global parameters for validation. In addition, they investigated laminar flame speed and Markstein length for iso-octane, n-heptane, toluene, different mixtures of Primary Reference Fuels (PRFs), Toluene Reference Fuels (TRFs), and three different gasoline fuels with three different RONs. All of their experiments were conducted in a constant-volume vessel at an initial temperature of 358 K, initial pressure ranges between 1 and 6 bar, and equivalence ratios between 0.8 and 1.6. They concluded that three different gasoline surrogates each consisting of different volume percentages of

iso-octane, n-heptane, and toluene have shown good agreement with the characteristics of real gasoline and hence can be used to mimic gasoline fuels.

Dirrenberger et al. [5] investigated real gasoline and a model fuel consisting of iso-octane, n-heptane, and toluene. The global parameter they used in their study was the adiabatic laminar burning velocity. The initial conditions used were 358 K and 1 atm. Different from the previously mentioned study, they conducted their experiments using a perforated plate burner. So, they used the heat flux experimental method, as opposed to what was used in [4]. Their focus was to study the aforementioned fuels and determine the effects of adding ethanol as an oxygenated additive. Their results revealed that there was no influence of adding ethanol up to 15% (vol).

The ethanol addition effect on a gasoline surrogate was studied by Yang et al. [6]. They performed laminar flame speed experiments to study a mixture of a gasoline surrogate plus ethanol. Their blend consisted of 23.33% iso-C_8H_{18}, 23.33% C_7H_8, 23.33% n-C_7H_{16}, and 30% ethanol. A spherical, constant-volume vessel was used for laminar flame measurements. The target global parameters were laminar flame speed and Markstein length. They have concluded that laminar flame speed is positively proportional to the initial temperature, while initial pressure and dilution ratio were inversely proportional to the laminar flame speed.

By looking at the literature for gasoline and its mixtures with ethanol, one can see a scarcity of laminar flame speed measurements, especially for high-ethanol-content mixtures, as stated by Pecchia et al. [3]. Therefore, the focus of the current study was to provide experimental data for laminar flame speeds of a gasoline surrogate and its mixtures with ethanol. Four different fuel mixtures consisting of the gasoline surrogate and ethanol were studied. The experimental procedure is presented next, followed by the laminar flame speed results for the gasoline surrogate and its mixtures with ethanol.

2   Experimental Setup

A heated, stainless steel, constant-volume vessel was used to conduct the current study. It has a cylindrical shape with a 31.8-cm internal diameter, 28-cm length, and 25.8-L volume. This vessel comes with two opposing glass windows with a diameter of 12.7 cm. A heating jacket, which can produce a uniform temperature up to 600 K, was used to heat the vessel for the desired temperatures. Three initial temperatures were investigated in this study, 335, 358, and 408 K. The vessel was designed for higher pressure. So, two initial pressures were investigated as well, 1 and 3 bar. A detailed description of the vessel can be found in Krejci et al. [7]. A modified Z-type schlieren imaging setup was used to capture the spherically propagating flame. A high-speed camera with a rate of 10,000 fps was used to capture the images. The collected images were then analyzed using an in-house Python code for edge detection. Laminar flame speed was then calculated using the non-linear equation developed by Chen [8].

The gasoline surrogate (E0), consisting of four components, namely, iso-octane, n-heptane, toluene, and 1-hexene, was premixed according to the McCormick blend [9]. Therefore, all components were mixed as follow: 55% iso-octane, 25% toluene, 15% n-heptane, and 5% 1-hexene by liquid volume. To investigate the effect of ethanol addition on the gasoline surrogate, three gasoline surrogate/ethanol mixtures were investigated. E30, E50, and E85 represent 30%, 50%, and 85% ethanol content in the mixture, while the remaining is the gasoline surrogate.

The fuel mixture was introduced into the vessel using an injection method. First, all components were premixed in a liquid phase with the specified percentages. Then the fuel mixture was injected directly into the vessel using a syringe with a known mass. The fuel mixture was allowed to fully evaporate, then air consisting of 21% oxygen and 79% nitrogen by volume was introduced into the vessel until the desired pressure was reached. The vessel pressure was monitored using a pressure transducer mounted on the vessel. The vessel temperature was also monitored using a thermocouple imbedded in the vessel.

3   Results and Discussion

The laminar flame speed for the baseline fuel (E0) used in this study was first tested at different initial conditions and compared to previously published data and a chemical kinetics model prediction. Then, the effect of ethanol addition on the laminar flame speed of the gasoline surrogate is presented. Finally, the gasoline surrogate/ethanol mixture from the current study (E30) was compared to results from the literature, where an overlapping set of conditions was available.

To validate the experiments, the gasoline surrogate (E0) studied in this paper was compared to real gasolines and a gasoline surrogate investigated by different groups. Figure 1 illustrates flame speed versus equivalence ratio for the current study compared to one gasoline surrogate studied by Mannaa et al. [4], and three different gasolines investigated by Dirrenberger et al. [5], Sileghem et al. [10], and Mannaa et al. [10], respectively. The gasoline surrogate investigated by Mannaa et al. is a mixture of 77.40% iso-C_8H_{18}, 17.6% n-C_7H_{16}, and 5% C_7H_8 which is different from the one used in the current study. Also, the initial temperature for all previously published data in Fig. 1 was 358 K, wherein in the current study the initial temperature was 359 K.

Moreover, the gasoline and gasoline surrogate data published by Mannaa et al. were obtained in a similar experimental setup using a constant-volume vessel, where spherical flame propagation was investigated. On the other hand, the other two gasoline flame speed datasets reported by Dirrenberger et al. and Sileghem et al. were obtained using heat flux experimental setups. Generally speaking, all data presented in Fig. 3 have the same pattern where the flame speed peaks near a 1.1 equivalence ratio. Both gasoline and gasoline surrogate flame speed data reported by Mannaa et al. show good agreement with the current study. However, gasoline flame speeds reported by the other two groups are faster than the current study's results by around 9.3% and 5.5% for Dirrenberger et al. and Sileghem et al, respectively.
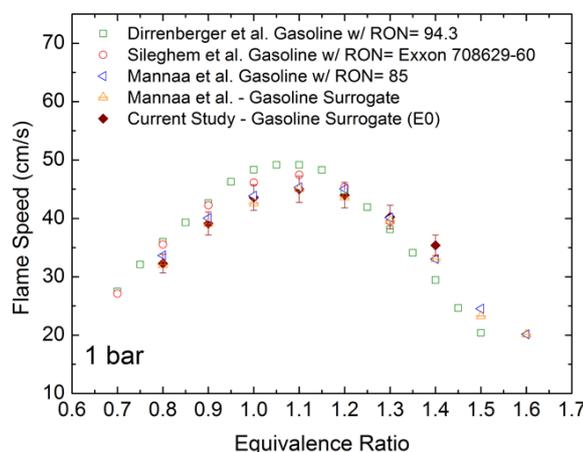
Figure 1: Laminar flame speeds of gasoline and gasoline surrogates for a range of equivalence ratios at 1 bar.

After establishing a good baseline fuel (i.e. gasoline surrogate E0), a study of the effect of ethanol addition was investigated to measure the laminar flame speed of different fuel mixtures of gasoline surrogate/ethanol. The following figures (Fig. 2(a)—Fig. 2(c)) illustrate the impact of ethanol addition to the gasoline surrogate. Moreover, ethanol addition impact was studied under different initial conditions (i.e. initial temperature and pressure). In addition, a chemical kinetics simulation was conducted to generate a prediction curve for the same initial conditions of interest. The mechanism of Mehl et al. [11] was used, and in this study is referred to as the LLNL model. Generally speaking, ethanol addition has enhanced the laminar flame speed of the gasoline surrogate under investigation at all initial conditions performed.

Figure 2(a) shows the laminar flame speed for E0, E50, and E85 at 1 bar and 335 K. It can be seen that as the ethanol content increases so does the flame speed. Following the usual behavior, the laminar flame speed peaks at rich to stoichiometric mixture at a 1.1 equivalence ratio. Adding 50% (by volume) ethanol (E50) to the gasoline surrogate (E0) has increased the laminar flame from 41.46 cm/s to 43.28 cm (at a 1.1 equivalence ratio), which is about 4.4% increment. As well, adding 85% (by volume) ethanol (E85) to the gasoline surrogate (E0) resulted in a 12.8% increase in laminar flame speed. In addition, increasing the ethanol content from 50% (E50) to 85% (E85) has enhanced the laminar flame speed by 8.09%, which is almost double than when increasing it from 0% to 50% (i.e. 4.4%). So, the laminar flame is more sensitive to higher ethanol content in this specific case. Also, model predictions by LLNL are presented in Fig. 2(a).

Figure 2(b) represents the laminar flame speeds for E0, E50, and E85 at 1 bar and 359 K. Again, increasing ethanol content resulted in an increment in the laminar flame speed. For example, at a 1.1 equivalence ratio, there was a 10. 6% and a 13.8% increase in flame speed for increasing ethanol content from 0 to 50% and 85%, respectively. However, at the same equivalence ratio, the flame speed was more sensitive to the addition of ethanol from 0% to 50% than the ethanol addition from 50% to 85%. Lastly, the LLNL model predictions are presented as solid lines in Fig. 2(b).

The effect of ethanol addition was also tested at higher pressure. Laminar flame speeds for E0, E50, and E85 at 3 bar and 359 K are presented in Fig. 2(c) along with predictions using the LLNL model. It can be seen as the ethanol content increases so does the laminar flame speed. Moreover, the laminar flame speed for all three fuel mixtures is peaking rich at a 1.1 equivalence ratio. In this higher-pressure case, the laminar flame speed increased by 4.6% after adding 50% ethanol (E50) to the gasoline surrogate (E0). While a 23.2% increase in laminar flame speed was reported after adding 85% ethanol (E85) to gasoline surrogate (E0). It also can be seen that the laminar flame speed was less sensitive to ethanol addition from 0% to 50% (increased by 4.6%) than the ethanol addition from 50% to 85% (increased by 17.8%) at a 1.1 equivalence ratio. One thing to note, the laminar flame speed of E85 at a 0.8 equivalence ratio was exactly equal to the one for E0. This result was the opposite of what was expected, where the laminar flame for E85 was always faster than the lower-ethanol content mixtures (i.e. E0 and E50). However, the model predictions in Fig. 2(c) show converging laminar flame speed for all three fuel mixtures when moving toward the lean side of stoichiometric; this can explain the drop in laminar flame speed for E85 at a 0.8 equivalence ratio.

(a)   (b)

(c)
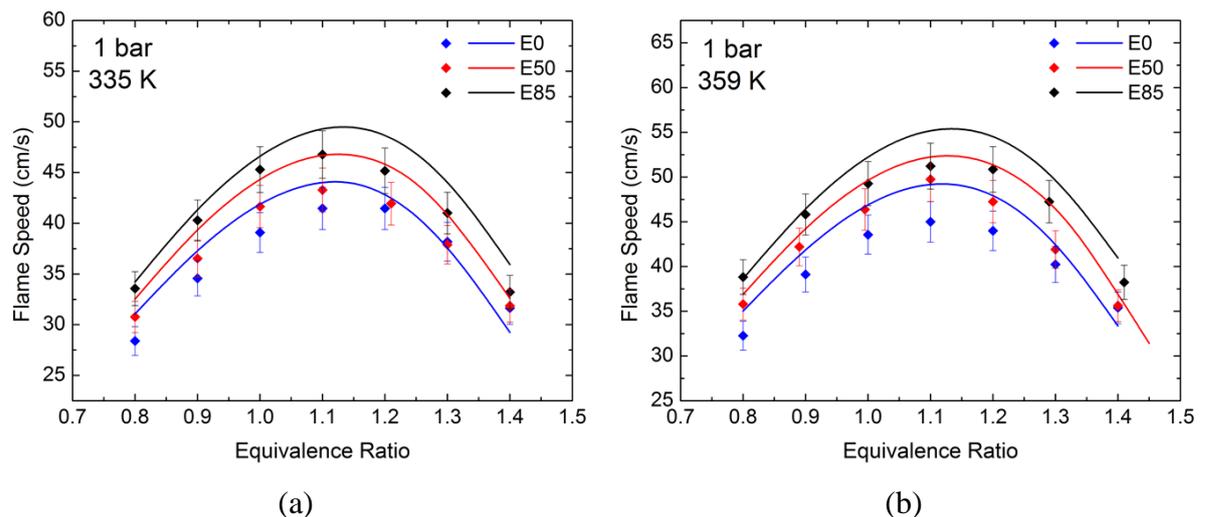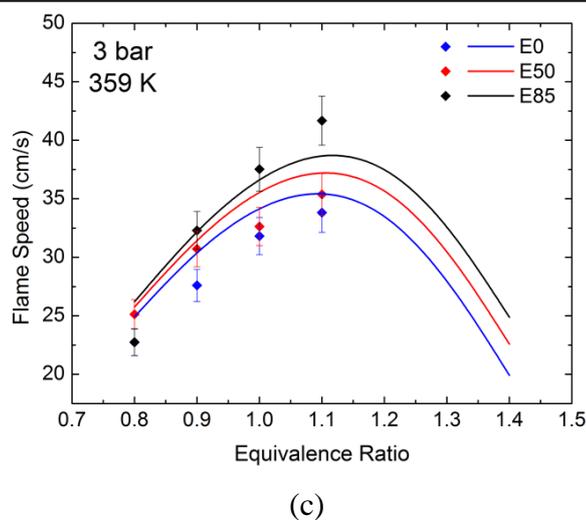
Figure 2: Comparison of experimental laminar flame speeds (symbols) and LLNL model predictions (solid lines) for E0, E50, and E85 at (a)1 bar and 335 K, (b) 1 bar and 359 K, and (c) 3 bar and 359 K.

Finally, the experimental laminar flame speeds for a gasoline/ethanol mixture (E30) produced in the current study are compared to previously published data in Fig. 3. In this figure, the laminar flame speed for E30 generated by Yang et al. [6] seems to be higher by 25.7% compared to the current study. In fact, Yang et al. tested their fuel in a small, constant-volume vessel with smaller glass windows (7.6 cm compared to 12.7 cm in current study) compared to the ones used herein. Also, they adopted a certain image selection criterion, where they only accepted a very narrow range of images (flame radii between 5 mm to 25 mm). Whereas in the current study, a broader range was covered (flame radii between 10 mm to 50 mm), given the freedom the larger windows provide. Furthermore, prediction results generated by the LLNL model seem to mimic the laminar flame speeds reported in this paper more closely.
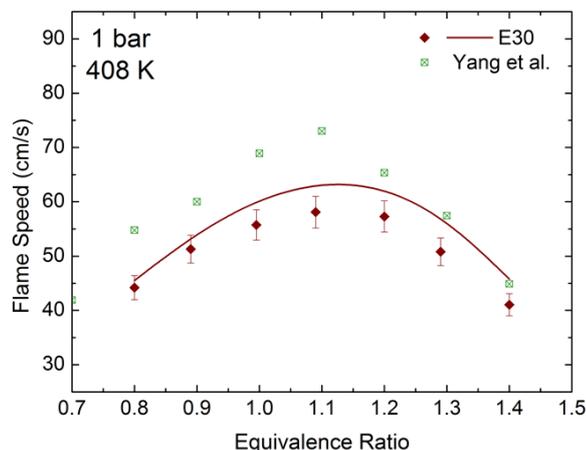
Figure 3: Comparison of experimental laminar flame speeds of E30 to the results of Yang et al.

4 Conclusion

An investigation of the effect of ethanol as an oxygenated additive to a gasoline surrogate was conducted, focusing on the laminar flame speed as the global parameter. During this investigation, four different fuel mixtures consisting of a gasoline surrogate and ethanol were examined. The current study concluded

that for the investigated gasoline surrogate/ethanol mixtures, the laminar flame speed peaks at an equivalence ratio of 1.1 for all investigated initial conditions. Furthermore, the results showed an increase in the laminar flame speed as the ethanol content increased over a range of equivalence ratios and fixed initial conditions. The current study was compared to the literature, with consistent results for E0 but some deviation for the E30 blend. Particularly, the E0 literature results with a similar experimental setup (spherical flame) showed stronger agreement compared to the results with the different type of experimental setup (heat flux method). Furthermore, prediction curves of laminar flame speed were generated using the LLNL kinetics model and were compared to the current study. These predictions were relatively higher by approximately 6%—12% for the whole range of equivalence ratios compared to the experimental results.

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