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Kinetic Modeling Study of Laminar Burning Velocity of Gasoline–Ethanol–Methanol Blends at Elevated Temperature and Pressure

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Abstract

Gasoline–ethanol–methanol (GEM) blends have been considered to replace pure gasoline as spark ignition engine fuel. Their physical and chemical properties and performance and emission measurements from real engines have been reported previously. However, a fundamental study that can explain the unique results of GEM compared with those of pure gasoline is lacking. This study aims to compare the laminar burning velocity of GEM blends at different mixtures, equivalence ratios, temperatures, and pressures with that of pure gasoline. A laminar flame propagation model and reaction mechanisms from the literature were used for a numerical simulation. In this study, the chemical components of real gasoline are simplified using a binary surrogate mixture. Results show that the laminar burning velocity of the GEM increased with the increase in temperature, ethanol, and methanol concentration, and it decreased with the increase in pressure. Sensitive reactions to laminar burning velocity are presented through a sensitivity analysis.

Keywords: gasoline–ethanol–methanol, kinetic modeling, laminar burning velocity

1. Introduction

Indonesian government has a policy for energy security, such as decreasing fuel import, especially for gasoline. The policy promotes the use of alternative energy sources, such as bioethanol [1] and methanol from coal and natural gas [2], as gasoline alternatives. Bioderived alcohol fuels such as bioethanol and biomethanol are considered a viable alternative to gasoline as a spark ignition (SI) engine fuel. Such fuels offer advantages over gasoline, such as cleaner burning and lower emission [3], and have been used as a binary mixture for gasoline. Recent trends show that a ternary blend of gasoline, ethanol, and methanol can be used as gasoline alternatives.

Bata and Roan [4] reported a study on GEM blends in 1989. They evaluated the exhaust emission of an OEM...
four-cylinder engine with different equivalence ratio and spark timing. Alcohols can reduce CO concentration up to 50% in the lean-stoichiometric side. Methanol was more effective than ethanol in reducing the CO concentration in exhaust gas. The drawback of the alcohol addition to gasoline is that it increased aldehyde concentration up to 60%–100%. The unburned hydrocarbon (UHC) reduction was not detected significantly in this study.

A main issue of the application of alternative fuels is the variation of fuel characteristics compared with conventional fuel, such as lower heating value, motor and research octane numbers (MON and RON), density, and air-to-fuel ratio. Turner et al. [5] proposed an iso-stoichiometric mixture for ternary blends of GEM. Thus, the resulting fuel characteristics are similar to those of E85 fuel (85 per cent ethanol and 15 per cent gasoline blend). However, a limiting zone exists where a mixture of GEM is unstable and cannot form a homogeneous mixture. Turner et al. [6] proposed an iso-stoichiometric GEM formulation to reproduce the gravimetric lower heating values, heats of vaporization, and molar concentrations of reactants in the charge, RON, and MON of any binary gasoline–ethanol blend. Furthermore, the engine performance and emission were evaluated in this study.

More studies reported the performance of GEM blends in engines. Pitcher et al. [7] observed the spray characteristics of two GEM blends and compared them with those of E85, methanol, and pure gasoline fuel using OH imaging and performed thermodynamic analysis. They found that the spray penetration of GEM blends was better than that of gasoline, methanol, and E85 fuels. Meanwhile, the highest peak pressure and pressure rise were found in gasoline and E85, respectively.

Sileghem et al. [8] reported the performance and emission tests of GEM blends on an SI engine. The addition of alcohols to gasoline results in lower burning temperature, NOx, and heat loss. The NOx emission of GEM blends was lower than that of gasoline but higher than that of methanol. Moreover, it improved the knock resistance and laminar burning velocity of the fuel. The engine performance measurements indicated that the GEM blends show significant efficiency improvement compared with gasoline. Meanwhile, different GEM concentrations have similar knock behavior and octane number.

Elfasakhany [9] compared the performance and emission of GEM blends with those of pure gasoline, ethanol, and methanol binary blends in an SI engine. Up to 10% alcohol in GEM blends yielded lower CO and UHC emission than in gasoline, but higher than in ethanol and methanol gasoline binary blends. The GEM blends exhibited moderate performance, and the highest and lowest volumetric efficiency, and the highest brake power were found in gasoline–methanol, gasoline, and gasoline–ethanol, respectively.

More engine tests on SI, homogeneous charge compression ignition (HCCI), and compression ignition engines were presented by Waqas et al. [10]. This study indicated that the iso-stoichiometric blending rule was valid for low concentrations of ethanol and methanol. At a higher ethanol and methanol concentration, the blending rule was not valid if a low RON gasoline was used. In HCCI combustion, the blending rule was not affected by the aromatics in the gasoline; the rule not valid for low RON gasoline, whereas it was valid for low and high speeds. For a high-temperature inlet, the blending rule was accurate and ethanol and methanol addition were less effective if high RON gasoline was used.

A 3500-km road test with 13 different GEM-fueled vehicles was performed by Schifter et al. [11]. This study reported that the use of oxygenated fuels was not effective in reducing emission in old vehicles, whereas similar fuel consumption and emission as pure gasoline were obtained. Amine [12] measured the distillation, vapor pressure, and octane number of binary and ternary GEM blends using ASTM-D86. Increasing the rate of blended alcohol decreased the distillation temperature, whereas methanol blends display a more significant reduction in distillation temperature compared with gasoline–ethanol blends. The distillation curve of ternary blend GE5M5 is placed in between the distillation curves of binary fuel blends GM10 and GE10. With similar alcohol concentration, the GEM blends have a higher octane number compared with the GE blend. A recent study by Waluyo et al. [13] discovered that ethanol addition to gasoline–methanol blends could assist the mixture in becoming homogeneous. Furthermore, engine performance tests were reported in this study.

Considering the idea of GEM blends as a gasoline alternative, studies on this fuel are limited to engine performance and emission test. This study aims to extend the study of GEM blends to the prediction of laminar flame speed at elevated temperatures and pressures, which has not been reported so far. Laminar burning velocity is an important fundamental combustion characteristic that represents the reactivity, diffusivity, and exothermicity aspects of the combustion process. It characterizes the speed of the flame front traveling toward unburned premixed gas. Understanding the characteristic of the laminar burning velocity of GEM blends may help explain the results of engine performance and emission tests that were reported earlier.
2. Methods

Laminar flame speed measurement is usually performed by observing the propagation of the flame front in a constant volume bomb, counterflow flame, or heat flux burner [14], [15]. Alternatively, a numerical method can be used to predict the laminar burning velocity of premixed gas mixtures. This application becomes possible with the availability of a freely propagating laminar flame, reaction mechanisms, thermodynamics, and transport models.

In this study, laminar flame speed calculation was performed using a Cantera–Python program developed previously [16]. The program requires an input of the reactor physical parameters and a reaction mechanism that consists of a set of elementary reaction, thermodynamic, and transport data of the species. The author tested the repeatability of the data that are generated by the code. The generated data are similar for similar settings and the simulation converges. The code for the freely propagating flame model is documented in the Cantera website [17][18].

Initially, Kee et al. [19] developed a FORTRAN program for modeling laminar premixed flame temperature and species profiles. The program can be configured to model freely propagating and burner-stabilized flames. In this study, the freely propagating flame model is selected to calculate the laminar burning velocity of the fuel mixtures, and provides the species profile and the adiabatic flame temperature by solving the energy equation, mass continuity, species reaction, and the equation of state, which are expressed as follows, respectively:

\[
\frac{d T}{dx} - \frac{1}{c_p} \frac{d}{dx} \left( \frac{d T}{dx} \lambda \right) + \sum_{k=1}^{K} \rho Y_k V_k \frac{d}{dx} \left( V_k \right) + \sum_{k=1}^{K} \dot{\omega}_k h_k W_k = 0 \quad (1)
\]

\[
\dot{M} = \rho u A \quad (2)
\]

\[
\dot{M} \frac{d Y_k}{dx} + \frac{d}{dx} \left( \rho A V_k \dot{Y}_k \right) - A \dot{\omega}_k W_k = 0 \quad (3)
\]

\[
\rho = \frac{\dot{W}}{RT} \quad (4)
\]

where \( \lambda \) is the thermal conductivity of the mixture \( \dot{M} \) is the mass flow rate, \( \dot{W} \) is the average molecular weight of the mixture, \( V_k \) is the diffusion velocity of the \( k^{th} \) species, and \( \dot{\omega}_k \) is the production rate of species \( k \), which is determined by solving the chemistry data using the forward Arrhenius coefficient and Eq. (5) including the pressure-dependent reaction. The thermodynamic data in NASA polynomial format are used to provide the value of heat capacity, enthalpy, and entropy of the species in a wide temperature range. The transport data, which consist of collision parameter, polarizability, dipole moment, and rotational relaxation, are also provided. PREMIX is now part of the CHEMKIN package, which is licensed under ANSYS. As an open-source alternative to CHEMKIN, Cantera is introduced with similar modeling capabilities.

\[
k = AT^n \exp\left(\frac{-E_a}{RT}\right) \quad (5)
\]

The challenge of modeling gasoline reaction is that real gasoline consists of many hydrocarbon molecules. To simplify the chemical composition of a real gasoline, a surrogate mixture is used based on the work of Stagni et al. [20]. The surrogate consists of n-heptane, iso-octane, and toluene with mole fractions of 63%, 20%, and 17%, respectively. The surrogate formulation was reported to be able to mimic the physical and chemical properties of real gasoline. The reaction mechanism from Stagni et al. [21] is also used to model gasoline surrogate and the GEM blends. The reaction mechanism consists of 3,370 reactions among 156 species, including low-temperature reactions. This mechanism was validated against experimental data such as laminar flame speed and species concentration from several reactors. Thus, this mechanism is relatively accurate for modeling the gasoline surrogate and is a reduced mechanism, thus, it can save computational resources while maintaining accuracy.

The fuel mixtures that were simulated for the laminar burning velocity in this study are summarized in Table 1. The ethanol and methanol concentrations in the fuel samples were selected to identify the effect of ethanol and methanol on the laminar burning velocity of the fuel blend when they are dominant and similar in the GEM blends. Gasoline is also included as a benchmark of the conventional fuel. If the concentration of ethanol and methanol is too low, then the change in the laminar burning velocity is less noticeable. The fuel-to-air ratio is expressed as an equivalence ratio, which is formulated as follows:

\[
\phi = \frac{\left( \frac{n_{fuel}}{n_{air}} \right)_{reaction}}{\left( \frac{n_{fuel}}{n_{air}} \right)_{stoichiometric}} \quad (6)
\]

where \( n \) is the amount of fuel or air in mole, whereas the theoretical air is used for the model. For each fuel mixture, 36 equivalence ratios were simulated from 0.6 to 1.5.
<table>
<thead>
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<td>Ethanol</td>
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The reactor temperature is set at 373 K, 423 K, and 473 K at 0.1 MPa to understand the effect of temperature variation on the laminar flame speed of the fuel blends. Moreover, the reactor pressure is adjusted to 0.2 MPa and 0.5 MPa keeping the temperature constant at 473 K to observe the effect of pressure variation on the laminar burning velocity. Sensitivity analysis was performed to identify the sensitive reactions to the laminar flame speed at different fuel mixtures, temperatures, and pressures.

3. Results and Discussions

Figure 1 shows the results of the laminar burning velocity of gasoline and GEM blends at 373 K and 0.1 MPa. The variation of equivalence ratio affects the laminar burning velocity, which peaks at approximately \( \phi = 1.1 \) with 0.58 m/s. In a lean region below 0.8, the burning velocity of pure gasoline and GEM blends is relatively similar. In the region richer than 0.8, gasoline has a lower burning velocity compared with the GEM blends. The GEM blends have a similar burning velocity in the lean region up to the stoichiometric. In the rich region, the difference between the GEM blends becomes more noticeable. The highest burning velocity is achieved by the blend with a higher methanol concentration, whereas the burning velocity of the GEM blends is decreased by making the ethanol concentration higher than the methanol concentration. Meanwhile, the blend that has similar ethanol and methanol concentrations has a burning velocity in between that of the other GEM blends.

The higher burning velocity with more methanol concentration is caused by the higher burning velocity of methanol compared with ethanol, whereas gasoline has the lowest burning velocity [22]. These fuels have different chemical structures, where methanol has the simplest structure and gasoline has the most complex structure. The more complex structure undergoes more reactions to break the bonds and forms combustion products, such as CO₂ and H₂O.

Figures 2 and 3 present the effect of temperature variation on the burning velocity of the fuels at 423 K and 473 K with 0.1 MPa. Compared with the results in Figure 1, increasing the temperature to 423 K increases the burning velocity of gasoline and GEM blend by approximately 0.1 and 0.13 m/s, respectively. The order of the highest burning velocity among these fuels does not change compared with that shown in Figure 1. A further temperature increase to 473 K increases the burning velocity of gasoline and GEM blends by approximately 0.15 m/s compared with the results shown in Figure 2.

Figure 1. Laminar Burning Velocity of Gasoline and GEM Mixtures at 373 K and 0.1 MPa

Figure 2. Laminar Burning Velocity of Gasoline and GEM Mixtures at 423 K and 0.1 MPa

Figure 3. Laminar Burning Velocity of Gasoline and GEM Mixtures at 473 K and 0.1 MPa
Figures 4 and 5 present the burning velocity of gasoline and GEM blends with the variation of reactor pressure at 0.2 and 0.5 MPa keeping the temperature constant at 473 K. Compared with the results in Figure 3, increasing the pressure to 0.2 MPa decreases the burning velocity of gasoline and GEM blends by approximately 0.1 m/s. The equivalence ratio where the burning velocity peak is located is relatively similar in all reactor conditions. A further pressure increase to 0.5 MPa results in a lower burning velocity compared with the results from 0.2 MPa, which is lower by 0.13 and 0.17 m/s for gasoline and GEM blends, respectively.

Sensitivity analysis was performed to identify reactions that are most sensitive to the laminar burning velocity using the Cantera–Python program. Different combination of reactor temperature and pressure keeping the equivalence ratio at stoichiometric levels was investigated using this program to determine any unique behavior from the sensitivity analysis. In all reactor conditions, the sensitive reactions to the burning velocity are relatively similar. Figure 6 presents 10 reactions that are most sensitive to the burning velocity at 473 K and 0.5 MPa, which is relatively similar to other combinations of temperature and pressure. In GEM blends and gasoline, the most sensitive reaction that increases the laminar burning velocity of the flame is $\text{H} + \text{O}_2 = \text{O} + \text{OH}$. The most sensitive reaction that decreases the laminar flame speed of the flame is $\text{H} + \text{OH} + \text{M} = \text{H}_2\text{O} + \text{M}$.

The prediction of the laminar burning velocity of GEM blends may explain the findings that were reported earlier. Pressure rise is directly proportional to the burning velocity and alcohol concentration and the premixed unburned gas mixture burns faster than pure gasoline. However, further study is required to validate the prediction with experimental data and identification of the effect of ethanol and methanol in GEM blends on the concentration of pollutant gas emission. Moreover, the ignition delay time can explain the influence of ethanol and methanol on the octane number of the blends.

4. Conclusions

In this paper, a freely propagating flame model was used combined with a reduced reaction mechanism of a gasoline surrogate available from the literature to predict the laminar burning velocity of GEM blends. The simulated reactor temperature varied between 373 K, 423 K, and 473 K, and the reactor pressure varied between 0.1, 0.2, and 0.5 MPa. The ethanol and methanol concentrations at the GEM blends were varied to facilitate the observation of the burning velocity when ethanol or methanol is dominant. The simulation was performed within a wide range of equivalence ratio. Results show that with the addition of ethanol and methanol, the burning velocity of GEM blends became higher than that of pure gasoline. The highest laminar burning velocity is found near $\phi = 1.1$ in all reactor conditions. A higher methanol concentration in the GEM blend has a higher burning velocity compared with the situation when the ethanol concentration is higher in the blend. The increase in the reactor
temperature increases the burning velocity, whereas increasing the pressure decreases the burning velocity of the fuels. The sensitivity analysis indicates that the reactions of small radical molecules mostly affect the burning velocity of all fuels under all reactor conditions.

References