

The role of citronella oil as a bio-additive on laminar burning characteristics of iso-octane

I Made Suarta^{*1)}, Adi Winarta¹⁾, Agus Dwi Korawan²⁾ and I. DG Ary Subagia³⁾

¹⁾Mechanical Engineering Department, Politeknik Negeri Bali, Badung, Indonesia

²⁾Mechanical Engineering, Ronggolawe College of Technology, Cepu, Indonesia

³⁾Mechanical Engineering Study Program, Udayana University, Denpasar, Indonesia

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Abstract

This study focuses on the laminar burning velocity of iso-octane fuel with a citronella additive. The main objective is to investigate and synthesize the composition of citronella bio-additive in iso-octane fuel and how it affects laminar burning velocity. Laminar burning velocity testing was conducted in a cylindrical explosion combustion chamber at constant pressure with six compositions (IC-0 to IC-5) at equivalence ratios (ϕ) of 0.8 to 1.2. Functional groups were examined by Fourier Transform InfraRed (FTIR) and volatility was characterized by Thermogravimetric Analysis (TGA). The IC-2 mixture increased the Research Octane Number from 92.0 to 92.3; whereas, the smallest decrease in laminar burning velocity was 4.8% compared to IC-0. TGA testing showed an increase in volatility in IC-2. Overall, the addition of low dose citronella bio-additives, especially IC-2, provided a moderate octane increase with a minimal reduction in laminar burning velocity and improved evaporation, supporting its potential as a practical bio-additive for spark ignition fuels.

Keywords: Bio-additives, Citronella, Fuel, Laminar burning velocity

1. Introduction

Fossil fuels play an important role in ambient air pollution and global warming, impacting climate change [1, 2]. Although replacing fossil fuels with renewable energy is widely recognized as a key strategy for protecting the environment and human health, many countries continue to subsidize fossil fuels [3, 4]. In several reviews regarding the use of fossil energy, almost 25% of energy is used for transportation [5, 6]. In the last twenty years, various efforts have been made to meet the ever-increasing need for this energy. Efforts have been made to conserve new energy sources but this is relatively difficult to do because it clashes with environmental conservation [7, 8]. People have become used to subsidized fossil fuel prices in the long term; therefore, it is important to have alternative policies, to encourage clean transportation, environmental protection, and public health. New renewable energies have been discovered; the use of waste vegetable oil as biodiesel fuel was studied by [9-11]. The production of diesel oil from coconut oil was carried out by [12]. The blending of basic fuels with natural substances that have the potential to improve the quality and quantity of petrol, has also been widely carried out.

In traditional gasoline engines, motor octane numbers are routinely used to describe fuel performance and the anti-knock behavior of fuel, namely Research Octane Number (RON), Motor Octane Number (MON), and octane sensitivity ($OS = RON - MON$). Substantial advances have been made in chemical kinetics in recent decades and several studies have attempted to provide a fundamental explanation of RON and MON. Low-temperature combustion (LTC) and compression ignition (CI) strategies have been proposed as alternatives to spark-ignition combustion. This is due to the efficiency of diesel and offers an alternative to conventional CI combustion with very low NO_x and particulate matter (PM) emissions. Laminar burning velocity (S_L) is a laminar pre-mix flame characterization parameter because it provides information on the physicochemical properties of combustible mixtures. Burning velocity is influenced by several factors, such as pressure, temperature, and fuel mixture composition (fuel type, equivalence ratio (ϕ), and components mixed in the fuel) [13-16]. Laminar burning velocity provides invaluable information regarding the combustion properties and underlying oxidation chemistry of the fuel. It is also an important parameter in the design of engines, burners, and other equipment where combustion occurs [17, 18].

Citronella (*Cymbopogon Nardus*) is a plant that has many benefits. Citronella has an active content of 51.5% citronellal ($C_{10}H_{18}O$), 12.8% citronellol ($C_{10}H_{20}O$), and 15.0% geraniol ($C_{10}H_{18}O$) [19]; it is a colorless nonpolar liquid. Essential oil (Citronella oil) is obtained through the distillation of the citronella. Other characteristics of citronella are that it easily dissolves and evaporates in fuel, and is environmentally friendly. Based on the results of research on citronella conducted by [20-23], it is known that citronella added to liquid fuel (in this case, gasoline), has a positive impact. It reduces the rate of fuel consumption, has low exhaust emissions, and is abundant, making it very suitable for use as a vehicle fuel additive. Developing chemical kinetic mechanisms for these surrogate species is a challenge, requiring validation against experimental ignition data across a wide range of engine-relevant temperatures, pressures, equivalence ratios and dilutions.

*Corresponding author.

Email address: suarta@pnb.ac.id

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Testing of citronella as a fuel additive has been carried out, both on diesel fuel and gasoline fuel. Citronella was added to diesel fuel by [20, 22] and the test results showed that there has been an improvement in the performance and quality of diesel fuel exhaust gas. In another test, the addition of citronella to gasoline was carried out by [23-26], resulting in fuel savings when the gasoline mixture was added with 0.1% v citronella and 0.1% v clove oil.

The results of Gupta's research using gasoline fuel mixed with bio-ethanol E5 (5%v bio-ethanol) showed a slight increase in fuel consumption [25]. According to the test results, the brake thermal efficiency of the E5 increased by 0.3%. According to emissions analysis, E5 at full load resulted in lower emissions of 1.55% carbon monoxide, 2.00% smoke opacity, and 39 ppm unburned hydrocarbon. The results of the Prahmana test using gasoline fuel mixed with 1%v citronella and 1%v eugenol showed a decrease in fuel consumption [21]. At a 43% engine load, the BA2 (gasoline RON 88 + citronella oil 0.1% v+ clove oil 0.1%v) mix achieved the best reduction in fuel consumption (33.33%) when compared to pure petrol gasoline RON 88. For this gasoline blend, the average reduction in fuel consumption was 18.54%. Despite having the lowest volumetric efficiency, when compared to other mixes, the BA2 blend produced superior thermal efficiency.

This study addresses gaps in knowledge by examining the combustion dynamics of iso-octane-citronella blends using detailed experimental analysis, including FTIR and TGA, to elucidate the physical interactions and thermal behavior of the mixtures. The novelty of this work lies in its focus on the effects of citronella bio-additives on laminar burning characteristics and key factors of flame stretch velocity influencing engine performance and efficiency through a rigorous physicochemical and thermogravimetric approach. Most studies add additives to fuel to investigate fuel consumption and emissions without analyzing the fuel's basic characteristics. Burning velocity is an important characteristic that describes flame propagation. This method is widely used in kinetic model validation and is closely related to engine performance [20-23]. This study bridges the gap between fuel characteristics and burning properties to determine the best mixture concentration between fuel and citronella additive. The unique contribution of this research is to provide a physicochemical explanation of laminar flame dynamics using experimental and spectroscopic analysis, compared to previous studies that discussed citronella bio-additives [20-22].

Referring to the state of the art, research is focused on the role of citronella oil bio-additives on the velocity of fuel burning (iso-octane). This research is interesting because it involves natural substances as boosters to increase the performance of iso-octane fuel, especially the burning velocity. The aim of the research is to investigate and synthesize iso-octane-citronella composition at burning velocity. Next, we evaluate the role of citronella bio-additives as a fuel burning velocity booster. The research method was carried out through quantitative experiments by testing composition variations between fuel and citronella oil bio-additives. The characteristics of iso-octane and citronella composition were analyzed using FTIR and TGA.

2. Materials and methods

2.1 Materials

This research uses citronella oil (*Cymbopogon Nardus*) produced by the Institute Atsiri of Brawijaya University, with a purity of 82.468% and a density of $0.8769 \text{ g}\cdot\text{mol}^{-1}$, as a bio-additive added to iso-octane liquid fuel. Citronella is a biological resource which is abundant in almost all regions of Indonesia and has the potential to be used as a bio-additive for liquid fuel for motor vehicles. Citronella oil is produced through an extraction process and contains 82.468% citronellal, 13.151% citronellol, and 4.381% geraniol. Due to its abundant potential and ease of production, citronella oil is a candidate for use as a fuel additive in an effort to maintain economic pricing [20, 21, 27]. In addition to being an additive, citronella also has potential in the pharmaceutical, food, and other chemical industries.

Citronellal, citronellol, and geraniol are compounds formed by the elements carbon (C), hydrogen (H), and oxygen (O). Citronellal ($\text{C}_{10}\text{H}_{18}\text{O}$) is a monoterpene with the oxygen content shown in Figure 1(a). Citronellol ($\text{C}_{10}\text{H}_{20}\text{O}$) (Figure 1(b)) is also called dihydrogeraniol, which is a natural monoterpenoid, while geraniol ($\text{C}_{10}\text{H}_{18}\text{O}$) (Figure 1(c)) is generally called rhodinol and is a monoterpenoid and alcohol compound.

Iso-octane was used as the sole substrate for gasoline fuel. The iso-octane used is produced by Merck, with the molecular structure: 2,2,4-trimethyl pentane, a molar weight of $114.23 \text{ g}\cdot\text{mol}^{-1}$ and a purity of 99.5%.

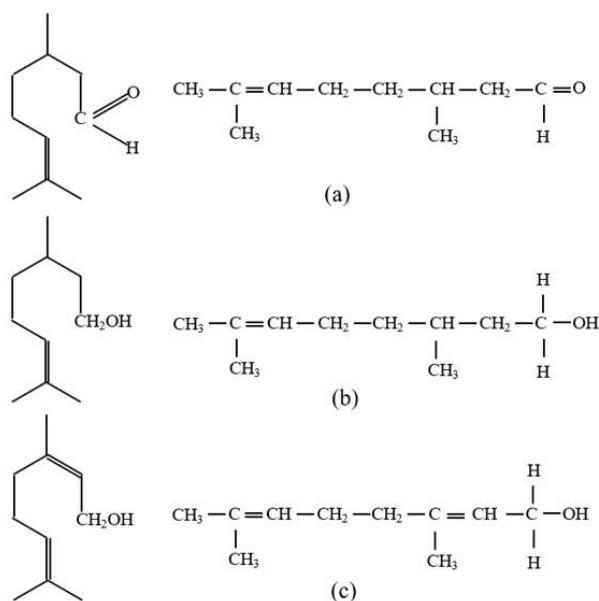


Figure 1 Structure and molecular bonds of monoterpenes (a) Citronellal, (b) Citronellol, (c) Geraniol

2.2 Manufacturing process

The basic characteristics of the fuels tested are shown in Table 1. These characteristics are very important for analyzing the characteristics of the mixture that occurs and its combustion.

Table 1 Test fuel properties

Properties	Iso-octane [27]	Citronella
Purity (%)	99.500	82.463
Chemical formula	C ₈ H ₁₈	C ₁₀ H ₁₈ O
Boiling Temperature (°C)	98.00-100.00	97.86 [22]
Enthalpy of evaporation at 25°C (kJ·kg ⁻¹)	308.00	44.22 [22]
H/C ratio	2.25	1.80
O/C ratio	0.0	0.1
Low heating value (MJ·kg ⁻¹)	44.4	41.4 [26]
Flash point (°C)		94 [28]
Fire point (°C)		100 [26]
Molecular weight (g·mol ⁻¹)	114.23	154.00
Density (kg·l ⁻¹)	0.6910-0.6960	0.8769
Vapor pressure at 20 °C (kPa)	5.50000	0.03733 [29]
Oxygen content (wt%)	0.00	10.39

Table 2 shows the mixture variations. Each composition was tested at equivalence ratios (ϕ) of 0.8, 0.9, 1.0, 1.1, and 1.2. The equivalence ratio is the ratio of actual air to fuel to the stoichiometric fuel ratio. The composition of the iso-octane and citronella bio-additive mixtures was carried out in five variations, with the mixture compositions being in v/v% units. The concentration range (0.1–0.5% v) was selected based on previous studies [22, 23], showing optimal performance and fuel savings at citronella concentrations of 0.10–0.15%. This range ensured observable physical and chemical effects without altering the fuel phase stability.

Table 2 Citronella blend composition versus iso-octane substance

Mixture	Code	Citronella (%V)	Iso-octane (%V)	Equivalence ratio (ϕ)
I	IC-0	0.00	100.00	0.8; 0.9; 1.1; 1.2
II	IC-1	0.10	99.90	
III	IC-2	0.15	99.85	
IV	IC-3	0.20	99.80	
V	IC-4	0.30	99.70	
VI	IC-5	0.50	99.50	

IC= iso-octane and citronella composition

2.3 Test equipment

The burning velocity test was conducted in a cylindrical explosion combustion chamber. The cylinder had a diameter of 135 mm and a length of 350 mm, as shown in Figure 2. This model was used by [30]. One end of the combustion chamber was closed with a transparent glass wall, to record the flame growth video with a high-speed camera. The other end had a piston that could move freely during the development of the fireball.

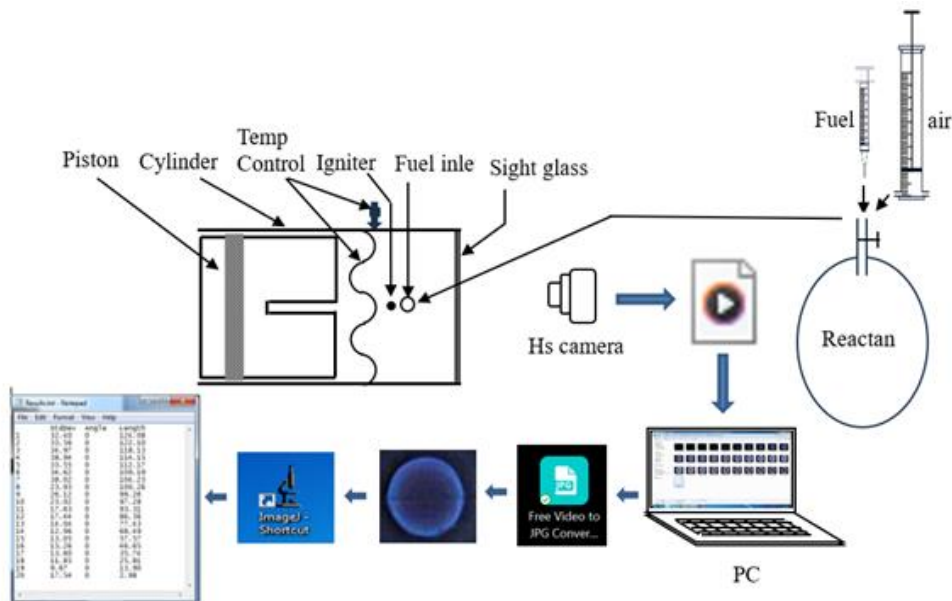


Figure 2 Test equipment

The left-hand-side wall of the cylinder was equipped with a positive (+) terminal from the igniter and an inlet for entering the reactants. The right-hand-side wall was installed with a negative (-) terminal from the igniter and a scavenging manifold. The igniter had an energy of 0.26 MJ. Mixing of the air and fuel was carried out in a mixing bag. The ratio of the volume of air to fuel entered into the mixing bag was measured based on the Air Fuel Ratio (AFR) of each fuel with its additive composition. The burning speed test was tested at equivalence ratios (ϕ) of 0.8, 0.9, 1.0, 1.1 and 1.2, where the equivalence ratio is $AFR_{actual} / AFR_{stoichiometric}$. $\phi < 1$ represents a lean mixture, $\phi = 1$ is a stoichiometric mixture and $\phi > 1$ is a rich mixture. The mixture was introduced into the combustion chamber through the fuel inlet. Before the igniter was ignited, the high-speed camera was turned on and set at a speed of 420 fps, with a resolution of 224×168 pixels. Calibration was performed using a 35 mm reference grid. Testing was conducted at atmospheric pressure and a temperature of approximately 302 K. The captured video was extracted into images and the flame diameter in the images was measured (using a program) to obtain the burning velocity.

2.4 Combustion analysis

In the burning test carried out, a spherical flame was captured by the camera. Next, the diameter of the spherical flame was measured at constant pressure, namely 1 atm. The equation used to measure the stretched flame propagation speed is the S_s equation, as shown in Eq. (1) [17, 31].

$$S_s = \frac{dr}{dt} \quad (1)$$

where r is the surface radius of the spherical flame front and t is the time when the diameter of the spherical flame was measured. Meanwhile, the stretched rate (α) of the spherical flame was calculated using Eq. (2), $\alpha = \frac{d(\ln A)}{dt} = \frac{\frac{1}{A} dA}{dt} = \frac{dA}{A dt}$ where A is the surface area of the spherical flame. In the case of a spherical propagating flame, the flame stretch rate can be calculated by the equation:

$$\alpha = \frac{dA}{A dt} = \frac{2}{r} \frac{dr}{dt} = \frac{2}{r} S_s \quad (2)$$

where (S_s) is a stretched flame speed and (S_n) is the unstretched flame speed. The linear relationship between the equations is shown in Eq. (3).

$$S_s - S_n = L_b \cdot \alpha \quad (3)$$

If the value of $\alpha=0$, there is an unstretched flame speed in Eq. (3) and the unstretched flame speed (S_n) is the same as the value of the stretched flame speed (S_s).

Next, the laminar burning velocity (S_L) was calculated from the derivative of the S_n equation shown as Eq. (4), namely:

$$S_L = \frac{\rho_b}{\rho_u} S_n \quad (4)$$

where ρ_b and ρ_u are the density of the combustion gases and the density of reactants, respectively.

2.5 Research octane number

The Research Octane Number (RON) is the quality of the gasoline fuel. RON affects the fuel's resistance to the combustion process in the engine. Fuel with a higher RON number value tends to have better resistance to knocking or detonation.

2.6 Fourier Transform Infrared Spectrometer (FTIR)

The Fourier Transform Infrared Spectrometer (FTIR) is a non-destructive technique for sample testing, which focuses on analyzing functional groups from solid or liquid materials using the ATR (Attenuated Total Reflectance) method. The results are obtained in the form of absorbance or transmittance graphs. FTIR type Prestige-21, from the joint laboratory of FMIPA Udayana University, was used to detect the functional groups formed. The detection range was determined based on the wavelength, in units of $1 \cdot \text{cm}^{-1}$, and transmission analysis, in % units.

2.7 Thermogravimetric analysis (TGA)

Thermogravimetric analysis (TGA) testing was carried out to test the thermal characteristics of the iso-octane and citronella fuel mixture. TGA is intended to determine the characteristics of a material against heat through changes in weight as a function of temperature or time. The sample was heated by increasing heat at certain intervals (referred to as dynamic measurement) or directly heated to a certain and constant temperature (isothermal measurement). Samples can also be heated to a nonlinear temperature, according to the program. The choice of temperature program depended on the type of information required about the sample.

3. Results

3.1 Laminar burning velocity

The laminar burning velocity is influenced by the equivalence ratio (ϕ), the heating value of the fuels, and the adiabatic flame temperature. When a mixture of fuel and air is ignited in the center of a combustion chamber, the flame will spread in a radial direction from the igniter to the reactants. Figure 3 shows an example of the propagation of spherical flames in IC-0 and IC-2 (mm); $\phi = 1$, with an interval of 2.381 milliseconds (ms).

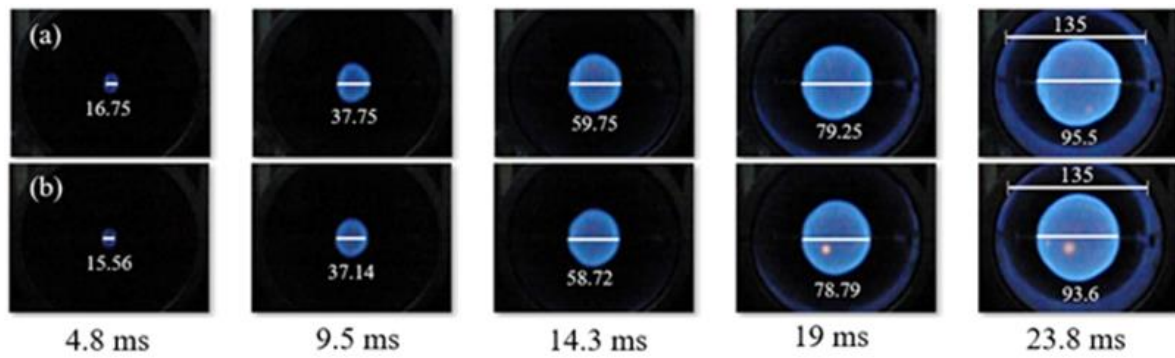


Figure 3 Propagation of spherical flame diameter (mm) of iso-octane and its mixture at $\phi=1$ (a) IC-0, (b) IC-2

Table 3 shows the results of the average flame diameter test at $\phi=1$ for IC-0 to IC-5, with four repetitions; a difference analysis was carried out using one way Anova (at a confidence interval of 95%). A p-value of less than 0.05 indicates a significant difference between IC-0 and IC-5 in Table 3.

Table 3 Test Results of one way Anova: IC-0 to IC-5 at $\phi=1$

Code	n	Mean	SD	F	p
IC-0	4	45.63	2.45	3.288	0.027
IC-1	4	36.65	8.69		
IC-2	4	41.78	5.09		
IC-3	4	37.13	8.02		
IC-4	4	34.04	7.65		
IC-5	4	28.47	5.49		

Figure 4 shows the flame diameter of iso-octane fuel mixtures with citronella at the mixture compositions of IC-0, IC-1, IC-2, IC-3, IC-4, and IC-5 at $\phi = 1$. These compositions were chosen based on the increase in calorific value and volatility. The test results for each mixture on the diameter of the formed round flame were measured until $t = 28.57$ ms. The test results show that, with the addition of citronella to the fuel, there is a linear decrease in the flame diameter. The diameter of the formed flame decreases accordingly, as shown for IC-0, IC-2, IC-1, IC-3, IC-4, and IC-5. The conclusion obtained from this test is that the addition of more citronella to the fuel has a negative impact on the flame diameter, which indicates inhibition of the burning velocity.

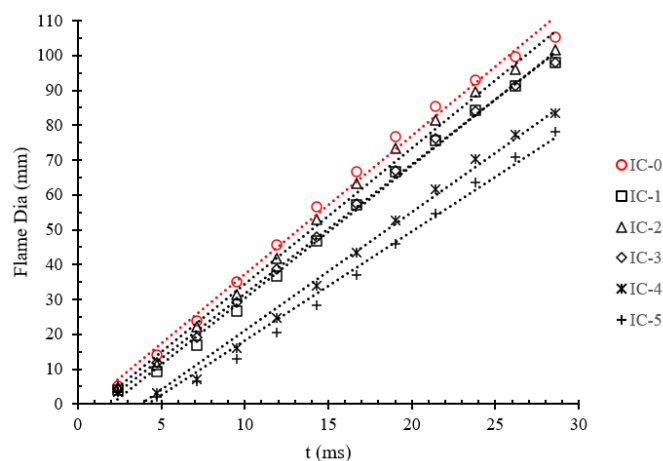


Figure 4 Comparison of the propagation of spherical flame diameter versus time

Figure 5 shows the stretched propagation flame speed of a mixture of iso-octane and citronella fuel at $\phi = 1$, which is calculated based on Eq. (3), the unstretched propagation flame speed is obtained when $\alpha = 0$. IC-0 is pure iso-octane, while IC-1, IC-2, IC-3, IC-4, and IC-5 are variations of the iso-octane-citronella mixture shown in Table 1. The test results showed that the stretched propagation flame speed of iso-octane is indicated by IC-0; whereas, after mixing citronella according to the ratio tested, there was a decrease in the stretched flame speed. The decrease occurred sequentially, thus: IC-2, IC-1, IC-3, IC-4, and IC-5. The initial ignition effect occurs up to $\alpha=0.28$ (1-ms^{-1}). After $\alpha<0.1$, the flame speed is influenced by the cylinder wall. Increasing the citronella composition reduces the cylinder wall effect. This is because a higher RON results in a more robust flame.

Figure 6 shows the laminar burning velocity (S_L) of iso-octane with citronella additive. The characteristics shown are that the best burning velocity occurs at $\phi = 1$. The next best burning velocity is at $\phi = 1.1$, then $\phi = 0.9$, then $\phi = 1.2$, and, finally, $\phi = 0.8$. Overall, the addition of citronella to iso-octane for each variation has the effect of decreasing the laminar burning velocity in a linear manner. At the IC-2 composition of all variations, there is the smallest decrease in burning velocity. The decrease in laminar burning velocity, due to the addition of citronella, occurs because citronella has a long molecular chain. Longer fuel molecules have a lower laminar burning velocity. Based on this characteristic, the addition of citronella is very suitable for use in engines with higher compression

ratios because it can increase the RON value. With these results, it was found that the iso-octane-citronella mixture is optimal at the IC-2 composition.

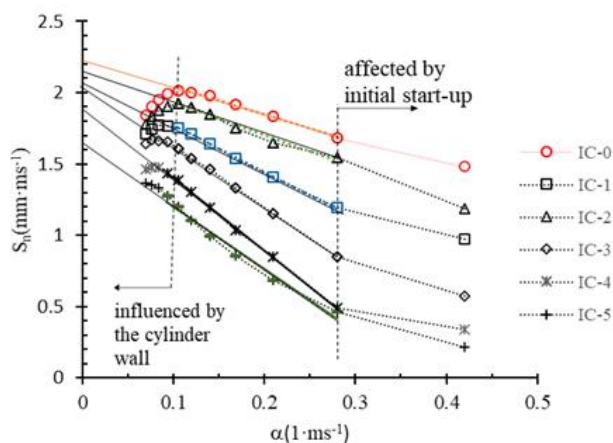


Figure 5 S_n value of iso-octane and its mixture at $\phi=1$

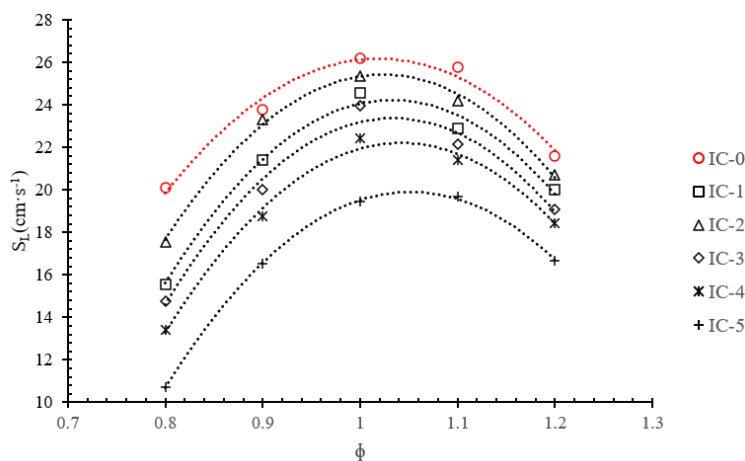


Figure 6 Comparison of laminar burning velocity of iso-octane fuel with added citronella mixtures

4. Discussion

4.1 Laminar burning velocity

By analyzing the results of the tests, which were carried out for the burning velocity of iso-octane mixed with various variations of citronella, the results showed a decrease in the laminar burning velocity. The successive decrease in burning velocity occurred in the compositions of IC-2, IC-1, IC-3, IC-4, and IC-5. This is because one of the basic characteristics of citronella is that it has a lower vapor pressure than iso-octane. The lower vapor pressure indicates that citronella is more difficult to evaporate than iso-octane, so the mixture of iso-octane and citronella fuel will reduce the burning velocity. The fuel burning velocity is influenced by density, viscosity, heating value, and volatility [30, 32].

Based on Table 1, the characteristics of iso-octane and citronella can be predicted. There are more carbon molecules from citronella than iso-octane, which indicates that it is more difficult to burn. The low heating value of citronella is lower than iso-octane, which reduces the burning velocity. The H/C of citronella is smaller than iso-octane, which indicates that the fuel will be more difficult to burn; however, the IC-2 mixture had the smallest decrease in laminar burning velocity. The largest increase in stretched burning velocity occurred at the initial start-up and increasing the citronella composition reduced the cylinder wall effect. This is because the higher RON results in a more robust flame. The addition of citronella increases RON, reduces cylinder wall effects, and makes the flame more robust. With this in mind, further testing of the characteristics of the iso-octane fuel mixture with citronella is needed.

4.2 Research Octane Number (RON) Test

RON testing (using the IKA/LEL-Octane-Cetane Analyzer) showed an increase in RON in iso-octane fuel after being mixed with citronella. Citronella increases RON and this is caused by the OH group, as in alcohol. Table 4 shows that the highest increase in RON occurred in the IC-2 mixture composition.

Although the increase in RON seems small, namely 0.3 points, it is important to improve engine performance because it can reduce the tendency for knocking at high compression. The addition of a combination of 0.1%v citronella additive with 0.1%v clove oil to RON 88 gasoline can reduce fuel consumption by 33.33% [21].

Table 4 RON of iso-octane fuel mixture with citronella.

Mixture	Code	Citronella (%V)	Iso-octane (%V)	Research Octane Number (RON)
I	IC-0	0.00	100.00	92.0
II	IC-1	0.10	99.90	92.1
III	IC-2	0.15	99.85	92.3
IV	IC-3	0.20	99.80	92.2
V	IC-4	0.30	99.70	92.2

IC= iso-octane and citronella composition

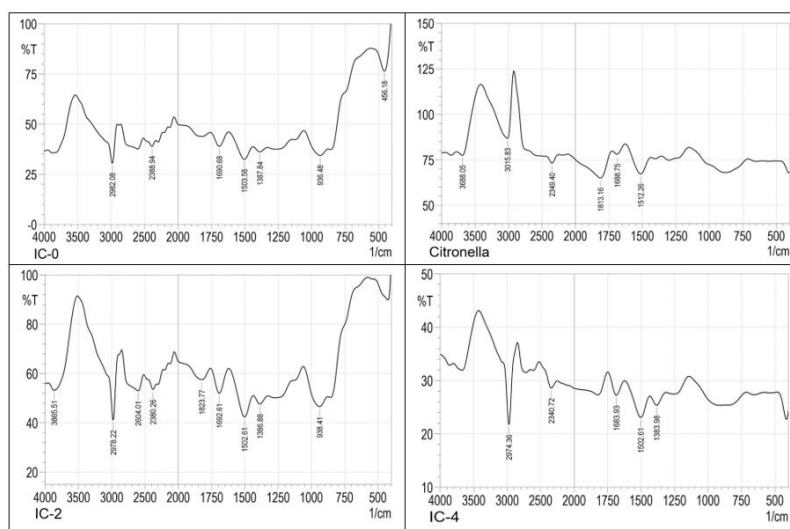
4.3 FTIR analysis

Based on Figure 7, the results of the FTIR test for iso-octane samples (IC-0) showed that there is a peak transmittance in the range 400–1500 cm^{-1} , which is the fingerprint region that shows the bending vibration of the C-C iso-octane atom. There is also a peak at 2982.08 cm^{-1} , which indicates C-H stretch.

In the FTIR test results for the citronella sample, transmittance was detected at 1688.75 cm^{-1} , which indicates the presence of C=O aldehyde. At 1813.16 cm^{-1} and 2349.4 cm^{-1} , it shows the presence of a C=C double bond and adsorption by C=O. The peaks 3015.83 cm^{-1} and 3688.05 cm^{-1} show the adsorption of a single bond C-H.

With the addition of citronella, changes were identified in the infrared transmittance pattern. The peak transmittance pattern of the mixture still resembled iso-octane in IC-2, and there was still a similar pattern in the fingerprint area.

When the citronella content was added to IC-4, the peak transmittance of the mixture of iso-octane and citronella changed, to become closer to the transmittance pattern of pure citronella, characterized by peak transmittance in the range 500–1500 ($1\cdot\text{cm}^{-1}$), which began to decrease. This is an indication of reduced bending vibration of the C-C iso-octane atom.

**Figure 7** FTIR test IC-0, citronella, IC-2 and IC-4

4.4 TGA analysis

Figure 8 shows the results of the TGA testing carried out on samples IC-0, IC-1, IC-2, IC-4, and citronella. The TGA test results show that there is a significant difference in mass reduction when citronella is added to IC-2. In the iso-octane sample, a mass reduction of 33.7% occurred at a temperature of 87.7 °C and, in the citronella sample, there was a mass reduction of 27.9% at a temperature of 147.5 °C. The addition of citronella at IC-2 resulted in a loss of 30% of the mass of the mixture at a temperature of 47.2 °C. This shows that the addition of citronella causes the sample to evaporate more easily. When the addition of citronella reaches IC-4, there is a decrease in the value of mass loss, as indicated by the mass reduction temperature of 30% achieved at a temperature of 77.93 °C.

These changes in properties are in accordance with changes in the FTIR peak transmittance pattern, which shows significant changes in the fingerprint region of IC-4, which more closely resembles the fingerprint region of citronella.

Based on the results of the IC-2 concentration of iso-octane and citronella mixing tests, there was a shift or change in the van der Waals bond between iso-octane molecules caused by the momentary dipole and the permanent dipole possessed by citronella. Citronella is polar but it also has long (nonpolar) hydrocarbon chains, this part can interact quite well with iso-octane through the London dispersion force. So there are two parts to the citronella molecule, namely the 'polar head' caused by one O atom and the 'long nonpolar tail' (C_{10} chain), this nonpolar part dominates the overall properties of the citronella molecule, so that citronella is somewhat nonpolar.

At higher concentrations of citronella additives, e.g. IC-4, more C=O bonds will give rise to more C=O bonds; its polar character increases so that the mixture will be closer to the Citronella graph.

In terms of chemical composition, the FTIR test results indicate that the mixture produces the same clusters. The TGA test showed similar thermal behavior, indicating no major chemical changes in the mixture. In terms of interaction, the FTIR test showed differences in absorption intensity, indicating compositional variation; whereas, the TGA test showed differences in evaporation rates, indicating the effect of the citronella composition. Both test results indicate the physical effect of the mixture. In terms of stability, citronella remained detectable in all of the samples. In the TGA test, citronella decreased the thermal stability of this mixture, indicating chemical consistency and thermal differences.

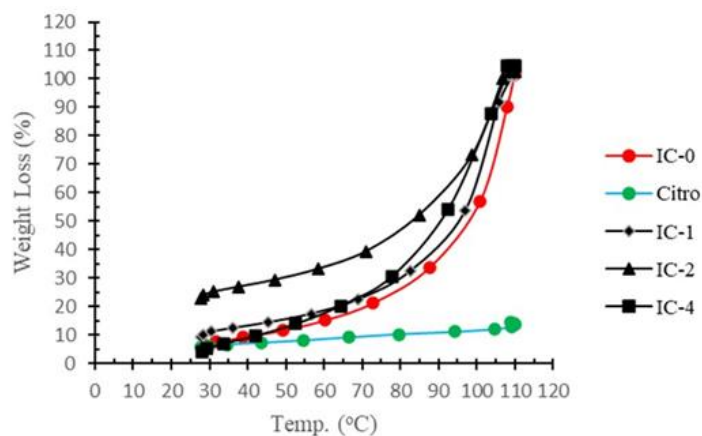


Figure 8 Graph of the relationship between weight loss and heating temperature

4.5 Molecular structure analysis

Figure 9(a) shows the molecular structure of iso-octane. Iso-octane is a non-polar saturated alkane compound with only van der Waals bonds occurring between its molecules. The bonds between iso-octane molecules are fragile dispersion forces [21, 33]. Figure 9(b) shows the structure of the citronella molecule. Citronella compounds have dipole-dipole bonds between their molecules and dipole-dipole interactions are stronger than dispersion forces.

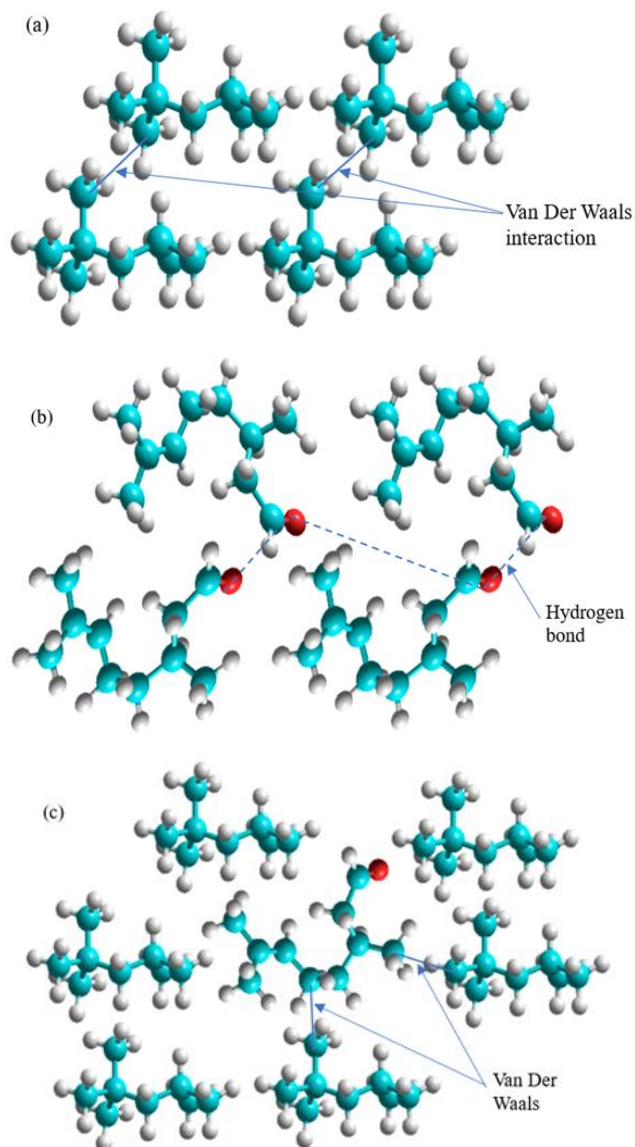


Figure 9 (a) Iso-octane molecular interaction, (b) Hydrogen bond in citronella, (c) Mixture of iso-octane molecules with citronella.

Figure 9(c) shows the molecular structure of the iso-octane compound mixed with citronella. Because the dispersion force of iso-octane is weaker than the dipole-dipole force of citronella, the citronella molecule easily inserts itself into the iso-octane molecule. When the citronella molecule enters the iso-octane molecule, it causes a shift in the arrangement of the iso-octane molecule. The IC-2 composition causes maximum molecular shift, with a minimum reduction in heating value. In a mixture composition of IC-2, each citronella molecule is surrounded by 710 iso-octane molecules. This composition causes interactions between cyclic citronella molecules and straight iso-octane molecules [34,35]. The addition of citronella molecules to iso-octane will shift the stability position of iso-octane, making it unstable and, therefore, flammable but reducing the calorific value. The uniqueness occurs in IC-2 because the molecular interaction produces a maximum molecular shift (the simulation in Figure 9c), which is supported by the FTIR test results (Figure 7) and the rapid evaporation rate (Figure 8) but without changing the heating value of IC-2, which approaches that of IC-0. Based on the test results, it can be concluded that maximum instability with the least reduction in heating value occurs in the IC-2 composition.

The presence of oxygen atoms in the citronella additive molecule is expected to increase the laminar burning velocity (S_L) but, in reality, the mixing results in a decrease in S_L and the smallest decrease occurs at the IC-2 concentration. This is caused by the long chain of citronella (C_{10}), which reduces the burning velocity. Citronella only has one O atom, which increases the laminar burning velocity.

4.6 Practical implications of the research

These findings have practical implications for the development of biofuel additives aimed at improving combustion characteristics in spark-ignition engines. The IC-2 blend, in particular, demonstrates the potential for applications in high-compression engines, where higher RON is beneficial, without significantly compromising combustion efficiency. The enhancements in flame propagation and ignition stability which were observed suggest that citronella oil can contribute to cleaner and more efficient energy conversion in internal combustion engines. In addition, this research supports the broader adoption of locally sourced, renewable bio-additives as a step towards energy diversification and environmental sustainability.

Burning velocity has implications for engine performance; high burning velocity is essential at high engine speeds. The combustion process is expected to generate maximum pressure several degrees after the top dead centre on the crankshaft and the fuel is completely burned before entering the exhaust manifold. Burning velocity affects combustion emissions in the combustion chamber. Complete combustion will produce CO_2 , H_2O , and N_2 emissions, which are considered harmless to the environment. Blending iso-octane fuel with citronella increases the RON value, which is beneficial for improving knock resistance. The testing of engine performance and emission quality will be conducted in future studies.

Due to its abundant potential and ease of production, citronella oil is a candidate to be used as a fuel additive in an effort to maintain economic fuel prices [20, 22, 25]. Apart from being an additive, citronella also has potential in the pharmaceutical, food, and other chemical industries.

5. Conclusions

The following conclusions can be drawn from this research:

1. Quantitative results show that the most effective addition of citronella to iso-octane, positively impacting laminar burning velocity, is composition IC-2.
2. The best citronella bio-additive composition for iso-octane is IC-2, which increases the RON value by 0.3 points.
3. Composition IC-2 lowers the evaporation temperature, thereby improving the homogeneity of the reactants in the combustion chamber.
4. Assessment of the mixture's lower heating value is needed; access to nearby laboratories which are equipped for this measurement is currently limited.
5. Further research needs to be conducted by blending citronella with ethanol to break down the long chains in citronella and increase the O_2 content in the fuel.

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