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Research article

The role of polar ethanol induction in various iso-octane ethanol fuel blend during single droplet combustion

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ABSTRACT

This study aims to disclose the role of molecular interactions of iso-octane ethanol blend during droplet combustion. The iso-octane ethanol composition which has the potential to form molecular clusters was analyzed using integer interaction modeling with mole ratio. Comparison of mole-based compositions was converted to a volume base to verify empirically using the single droplet burning method. The molecular interaction analysis gave the composition close to the molecular cluster composition was 10, 15, 25, 40, 50, 60, 70, 80, and 90% v/v. Ethanol fractions of 20% and 30% v/v were also tested using the same method as a mixture that do not form the molecular cluster. This study shows that the total molecular interaction forces on molecular clusters are inversely proportional to puffing events during single droplet combustion. The number of free molecules that do not form molecular clusters tends to produce micro-explosions at the final stage of single droplet combustion. The research also revealed that the increasing ethanol fractions in molecular clusters tends to reduce the combustion rate constant exponentially.

1. Introduction

The global need for fossil fuels continues to increase while the available reserves of conventional fuel reserves are depleting. Therefore, the attention of researchers to develop the role of alternative fuels shows increasingly close attention [1]. One of the significant concerns of researchers related to alternative fuels for the automotive sector is the use of bio-ethanol [2]. Ethanol can replace the role of gasoline and kerosene as fuel without significantly changing the existing main infrastructure. In-depth knowledge regarding the suitability of ethanol as an alternative fuel, especially in the automotive sector, is still a concern for researchers [3].

Research related to ethanol mixtures with conventional fuels has shown a prospective promise for the future [4]. The prospect of ethanol as a substitute for fuel because ethanol has valuable characteristics such as laminar flame propagation speed and higher-octane number compared to conventional fuels [5]. Ethanol substitution into conventional fuels also acts to increase the oxygen content of the fuel to produce complete combustion. The addition of ethanol to improve the octane quality of fuel is also believed to be able to reduce some pollutants of exhaust emissions [6].

However, most of the research on ethanol substitution with conventional fuels discusses the impact on engine performance [7,8], exhaust gas emissions [9–11], burning characteristic and engine behavior [12]. There are still rare studies that discuss changes in the properties of fuels such as vapor pressure [13], the stability of combustion flame [14], and the burning rate phenomena of combustion [15,16]. Several studies discussing the burning rate of substitution of ethanol with conventional fuels are carried out by analyzing single droplet combustion. Discussion of single droplet combustion is often associated with puffing and micro-explosion in droplets during the combustion process [17].

Burning rate is one of the properties of single droplet combustion which affects the power generated from the combustion process. The higher the burning rate constant of fuel tends to produce more power as well as. The fuel generated power (P) from its energy content was formulated by the following simple equation,

$$P = \frac{\Delta E}{\Delta t} \tag{1}$$

where ΔE is a change in energy from the fuel, and Δt is the time needed to change fuel energy. The burning rate constant of the droplet spacing can be explained by D^2-Law, which states that the square diameter of the droplet will be linearly reduced for combustion time [18]. Eq. (2) is the relationship between the constant burning rate (K) and the change in droplet diameter.

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$$D^2(t) = D_0^2 - K.\ t \quad (2)$$

where D is the final diameter of the droplet (mm), D_0 is the initial diameter of the droplet (mm) and K is the burning rate constant and t is the time (s). From Eqs. (1) and (2) above indicates that an increase in burning rate tends to produce higher power.

Molecular cluster is an aggregate of molecular units classified according to the strength of the interaction between molecules. The role of molecular and atomic cluster formation has long been theoretically investigated, such as in depositional events, liquid mixtures, and surface condensation and adsorption. An example of a molecular cluster between ethanol and water occurs because of a hydrogen bond. The ethanol-water molecule cluster produces new structures and energy levels [19]. Hydrogen bonding is the attraction between hydroxyl (OH) of ethanol and oxygen (O) of water. Hydrogen bonds of ethanol-water molecules produce strong relationships that cannot be separated by simple distillation [20].

Combustion of single droplets is one of the cheap and profitable analytical methods to characterize phenomena during the combustion process [21]. Combustion of the droplet is started with evaporation of the droplet, and then combustion occurs at the equilibrium line between the diffusion of the fuel vapor from the surface of the droplet and the diffusion of oxygen into the inside marked by a reaction on the outer flame with a certain distance from the droplet. Until now the discussion about constant burning rate (K) was only associated with micro-explosion and puffing events during the droplet burning process. While the polar ethanol mixture with non-polar gasoline (hydrocarbons) has the potential to build molecular clusters [22,23]. This molecular cluster occurs because polar ethanol induces non-polar gasoline (hydrocarbons) so that gasoline (hydrocarbon) changes to polar (induced dipole). Molecular interaction due to the attraction of the ethanol (permanent dipole) and gasoline (induced dipole) molecules is what contributes to the molecule cluster of hydrocarbons-ethanol blend.

Molecular interactions have a vital role in various physical, chemical and biological processes [24]. Molecular interaction is a force of attraction between two or more molecules or atoms that are not bound. Some examples of changes in molecular interactions occur in the process of smelting, boiling, sublimation, etc. that do not involve changes in bonds within the molecule. Explanation of the concept of molecular interaction can describe the character of various types of non-covalent bonds between molecules, and also describes the structural and other material characteristics. Although individually, the molecular interaction energy is small, cumulatively, it cannot be ignored [25].

This study aims to identify and explain the role of molecular interactions and molecular clusters with the incidence of puffing and micro-explosion during the droplet combustion process. This study used iso-octane (non-polar) as a representation of gasoline [26]. The iso-octane was used for it was a single substance, while gasoline was a multi-substance which simplifies the analysis of molecular interactions in the fuel blend.

2. Experiments

2.1. Fuel blends preparation

Iso-octane (2,2,4-Trimethylpentane) and ethanol (C_2H_5 OH) analytical reagent grade with a molar weight (MW) of 114.23 and 46.07 g $mole^{-1}$ and purity 99.5% and 99.7% respectively were used in this research. Ethanol was supplied by Smart-Lab, Indonesia, while iso-octane was supplied by Merck, Germany. Both fuels were used without additional purification. The fuel properties used in this study were presented in Table 1.

Iso-octane and ethanol used in this study refer to previous studies (10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, and 90% v/v) [22]. 15% and 25% v/v ethanol fractions were added because from analytical calculations has the potential to form molecular clusters, so this study uses ethanol fraction of 10%, 15%, 20%, 25%, 30%, 40%, 50%, 60%, 70%, 80%, and 90% v/v. Iso-octane and ethanol are were mixed manually in a reaction glass by stirring with a stirring spoon.

Table 1
Properties of test fuels.

Properties	Isooctane	Ethanol
Chemical formula	C_8H_{18}	C_2H_5OH
Purity (%)	99.5	99.7
Molecular weight (gram $mole^{-1}$)	114.23	46.07
Density @ 20 °C (kg L^{-1})	0.691–0.696	0.789–0792
Boiling temperature (°C)	98–100	78.3 [13]
Low heating value (MJ kg^{-1})	44.4	26.83
Enthalpy of evaporations at 25 °C (kJ kg^{-1}) [27]	308	924.2
H/C ratio	2.25	3
O/C ratio	0	0.5
Vapor pressure at 20 °C (kPa) [28]	5.5	5.95
Oxygen content (wt%) [28]	0	34.73

2.2. Experimental apparatus

Burning single droplets is an interesting analysis to examine the phenomenon of fuel combustion [21]. Experimental apparatus was designed to record the evolution of the droplet area of various iso-octane ethanol blends during combustion with a droplet. The evolution of droplet area per unit time was used to determine the burning rate which it was the physical properties of the fuel. While the incident during combustion (puffing and micro-explosion droplet) was recorded to revealed based on an intermolecular analysis between the constituents of each fuel mixture fraction. The experimental apparatus in this study were presented in Fig. 1.

The K type thermocouple wire with a diameter of 0.1 mm is stretched horizontally and supported by two supports as shown in Fig. 1. The temperature response of the thermocouple binder was in the form of an analogue signal in millivolts and then processed by TM4-N2RB to be converted into a digital signal. Digital signals were sent to personal computers via the RS 485 Autonics SCM-US481. Test data was displayed and stored on a personal computer using DAQ Master V1.6.3 software. Those that have been installed on a personal computer were set to pull the signal every 60 ms and stored in computer memory in the form of comma separated values (CSV) format files. CSV format files on personal computers were read with an excel program.

The thermocouple sensor was used as a droplet holder (droplet binder) to record temperature evolution during combustion of droplets (Fig. 1). A coil of nickel with a diameter of 0.5 mm was used as a heater to initiate combustion of the fuel mixture. High-speed video cameras were set to a certain distance and fixed to record droplet changes and consistently mix fuel droplet phenomenon.

2.3. Droplet fitting and capture

Single fuel droplet formation was done manually using conventional syringe (1 mL) with 100 strips showing the volume of liquid in the syringe so that each strip shows 10 μL (0.00001 L). Droplet size was set at a diameter of 1.0 ± 0.1 mm. The combustion initiation was used in the research of combustion of droplets was using nickel heating with a diameter of 0.5 mm with a 12 Volt 10 A DC power source. Heating control was carried out with a push on switch (push on switch) which simultaneously activates a high-speed camera to start recording the flame from burning droplets (Fig. 1).

2.4. Temperature and droplet area measurement

The evolution of the surface area of the droplet during the combustion process was recorded by a video camera (Fig. 1) with a speed of

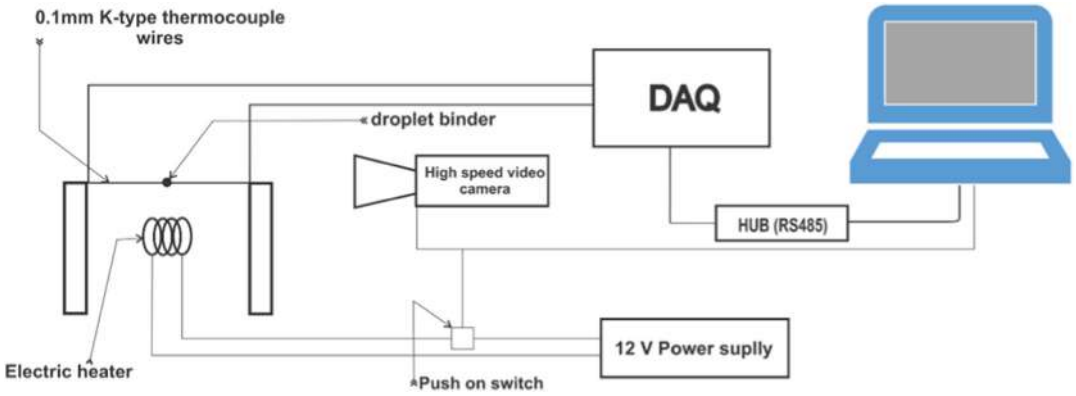

Fig. 1. Experiment apparatus.

20 frames per second (fps), it's means that every 1 s the droplet evolution video consists of 20 Image frames. Video were converted into images using video to JPG converter software. Diameter measurement during droplet evolution using ImageJ software bundled with 64-bit Java 1.8.0_112. The results of the measurement of the evolution of the droplet area during the burning process were plotted using origin 6.0 software to produce a clearer graphical display. While the evolution of the temperature during single droplet combustion was responded by a thermocouple binder forming a millivolt signal. This millivolt signal was processed by TM4-N2RB to be converted into a digital signal and connected to a personal computer via SCM-US481 RS 485 version. DAQ Master V1.6.3 Software. The DAQ Master V1.6.3 software installed on a personal computer was set to 0.050 s to pull data from the thermocouple signal. The temperature of the single droplet combustion test environment was conditioned at 25–27 °C. The temperature recorded by the thermocouple was a trend of temperature evolution during the combustion process of a single droplet. The close of flame to thermocouple binder had an impact on the temperature evolution reading of the droplet. The actual droplet temperature during the combustion process close to the boiling temperature of the fuel blend tested [29].

3. Result and discussion

3.1. Molecular cluster mole analysis

Molecular interactions are physical phenomena that are related to attraction and repulsion between molecules so that this interaction is related to the physical properties of a substance or a mixture of several substances. Ethanol is a polar liquid because it has a hydroxyl (OH) group at one end of its carbon chain. This hydroxyl group has a partial charge $\delta^+ = 0.209$ and $\delta^- = -0.395$ [22]. The difference in electronegativity (> 0.5) is what causes ethanol to have a permanent dipole while iso-octane is non-polar because it only has a partial charge (< 0.04) that is spread evenly on each of its constituent atoms. Ethanol iso-octane molecular interaction happen because the polar molecule of ethanol induces an iso-octane molecule, so there is a dipole-induced dipole interaction. The interaction of polar alcohol molecules with non-polar hydrocarbons, has the potential to form molecular clusters that have different physical properties with their corresponding molecules [22]. According to Table 1, it is known that the molecular weights of ethanol and iso-octane are 46.07 g.mole^{-1} and 114.23 g.mole^{-1} respectively, with the density at room temperature and pressure of 0.792 kg. L^{-1} and 0.696 kg. L^{-1}, respectively. Calculation of mole (n) of ethanol and iso-octane blends using Eq. (3) below,

$$n = \frac{Mr}{m} \tag{3}$$

where Mr is the relative molecular mass and m is the mass of the fuel. While the calculation of the volume (V) is determined by the following Eq. (4),

$$V = \frac{m}{\rho} \tag{4}$$

where ρ is the density of each fuel. Molecular interactions analysis is based on the concept that the number of interacting molecules is an integer, so the analytical calculation of the potential for molecular cluster formation due to the interaction of molecular iso-octane ethanol was presented in Table 2 below.

Table 2 above shows that all the mixture fractions have the potential to form molecular clusters except 20 and 30% v/v of the mixture fractions. The 15% v/v ethanol mixture fraction showed the lowest fraction error while 50% v/v ethanol mixture was the highest. The error fraction blend in forming molecular clusters in Table 2 shows the percentage of free of iso-octane or ethanol molecules outside the clusters. While molecular clusters of polar ethanol mixtures and non-polar iso-octane (hydrocarbons) produce different physical properties with their constituents. This error fraction causes two boiling points in the iso-octane ethanol mixture.

3.2. Evolution of droplet diameters of various iso-octane ethanol fuel blends

In this study single droplet of various fuel blends is placed on the unfolded thermocouple binder as in Fig. 2. The thermocouple wire is used to place doplets and simultaneously measure droplet temperature. The burning rate constant (K) is the slope of evolution of the diameter squared droplet change to time, which is denoted in Eq. (5) [30].

$$K = \frac{d}{dt}(D^2) \tag{5}$$

The evolution of the droplet diameter of each blend is recorded until the end of combustion. Micro-explosions are the phenomenon of

Table 2
Analytical iso-octane ethanol fractions that have the potential to form molecular clusters.

Mole iso-octane	Mole ethanol	Ethanol fraction v/v (%)	Ethanol fraction approach v/v (%)	Error fraction
3	1	10.5658	10	0.56585
2	1	15.0535	15	0.05350
–	–	–	20	–
1	1	26.1678	25	1.16783
–	–	–	30	–
1	2	41.4810	40	1.48099
1	3	51.5332	50	1.53323
1	4	58.6382	60	1.36175
1	7	71.2723	70	1.27231
1	12	80.9635	80	0.96354
1	25	89.8586	90	0.21048

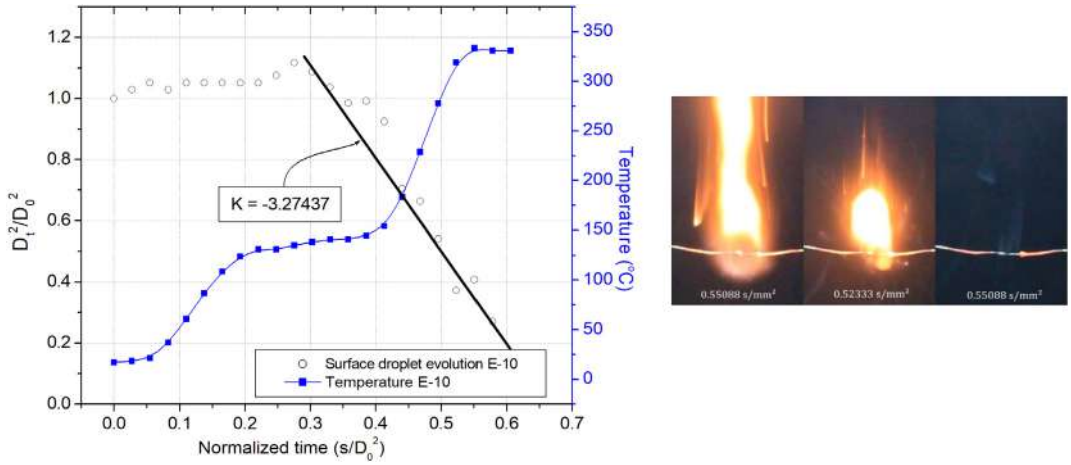

Fig. 2. Single droplet combustion of 10% v/v ethanol fraction blend.

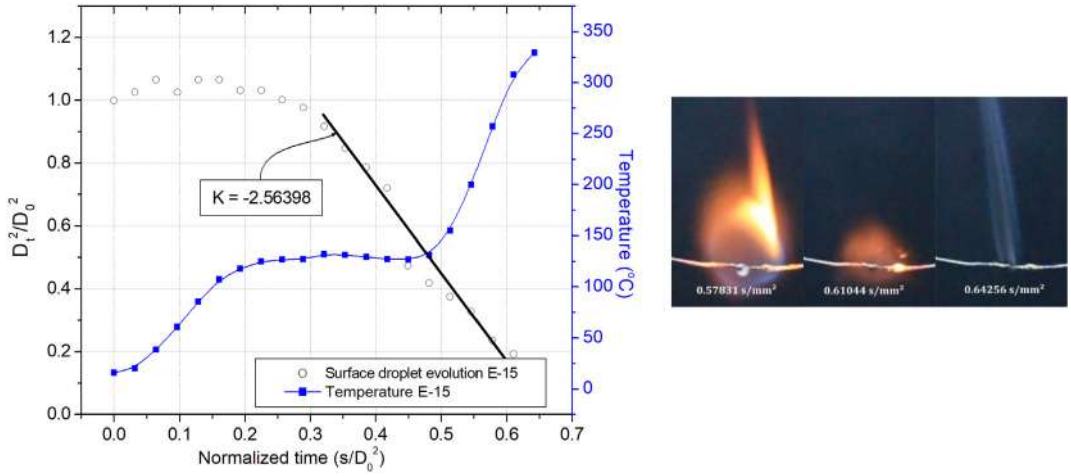

Fig. 3. Single droplet combustion of 15% v/v fraction blend.

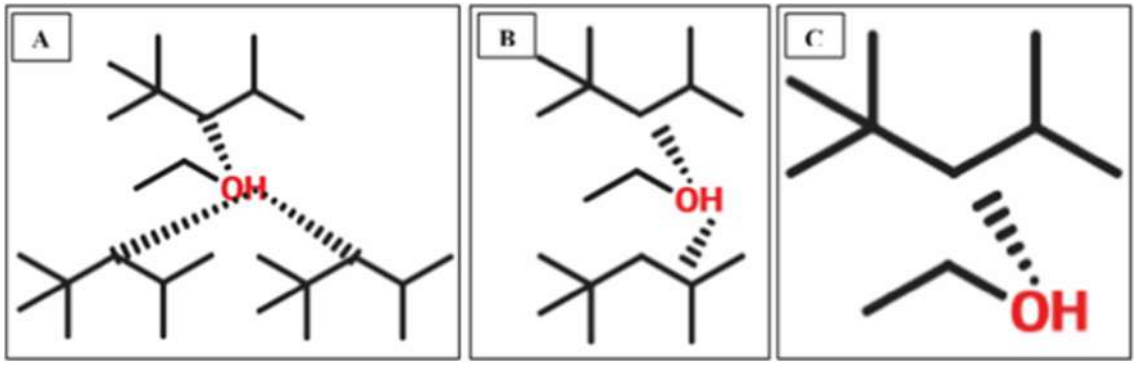

Fig. 4. Molecule model of ethanol iso-octane cluster, A: 10.5658% v/v; B: 15.0535% v/v, C: 26.1678% v/v.

breaking a part or all of the droplet, while puffing is expanding the droplet but not breaking. The micro-explosion will atomize droplets which help improve combustion efficiency [31].

Droplet combustion for ethanol fraction 10% and 15% v/v (low fraction) shows the same behavior, especially in the first stages and the final stage of combustion of droplets as shown in Figs. 2 and 3. At the first stage, puffing droplet occurs up to 0.3 unit of normalized time. In the low fraction ethanol blend, the number of non-polar iso-octane molecules is higher than polar ethanol molecule. So, due to the intermolecular force within the cluster of molecular models is so weak (Fig. 4) that it tends to produce a long regime puffing droplet at the first stage of droplet fuel blend combustion (Figs. 2 and 3). In the final stage of combustion of a single low fraction droplet (Figs. 2 and 3), observations show that burning of the fuel blend is swift. The speed of combustion of droplets at this final stage is due to iso-octane having a high LHV (Table 1) so that it has an impact on the high rate of droplet evaporation of the fuel blend.

Fig. 4A and B shows that the fraction of ethanol mixture is 10.5658%, 15.0535% v/v. One molecule of ethanol induces three and two iso-octane molecules respectively. So, one partial charge of the ethanol hydroxyl group has the burden of inducing three and two iso-octane molecules, so that the interaction forces on this side are weaker

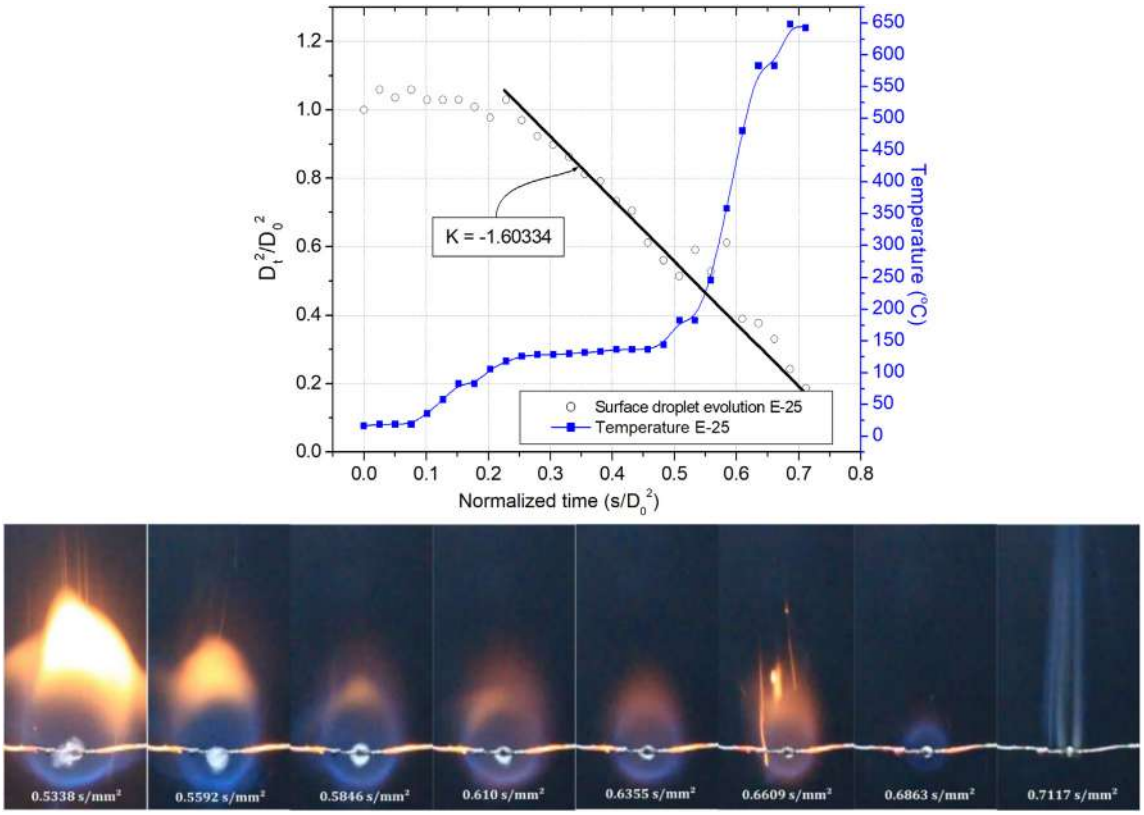

Fig. 5. Single droplet combustion of 25% v/v fraction mixture.

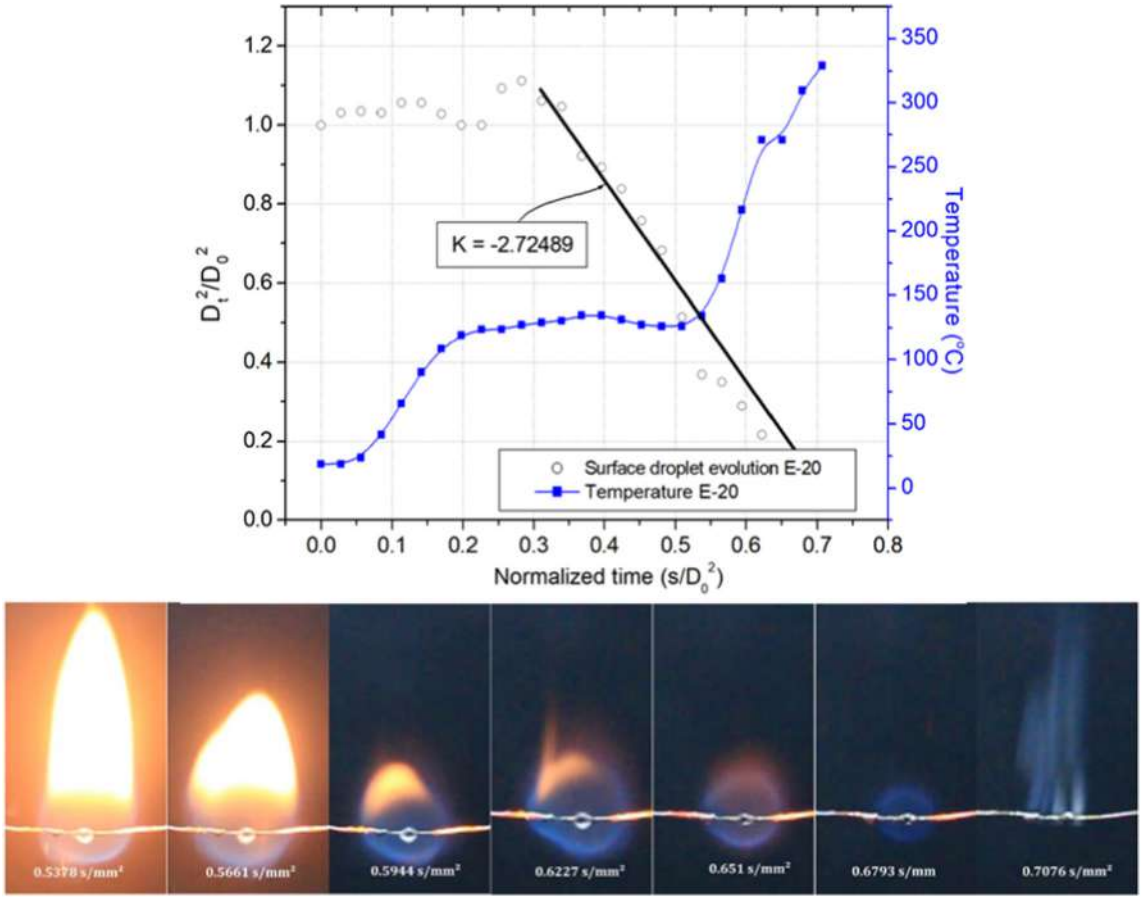

Fig. 6. Single droplet combustion of 20% v/v fraction mixture.

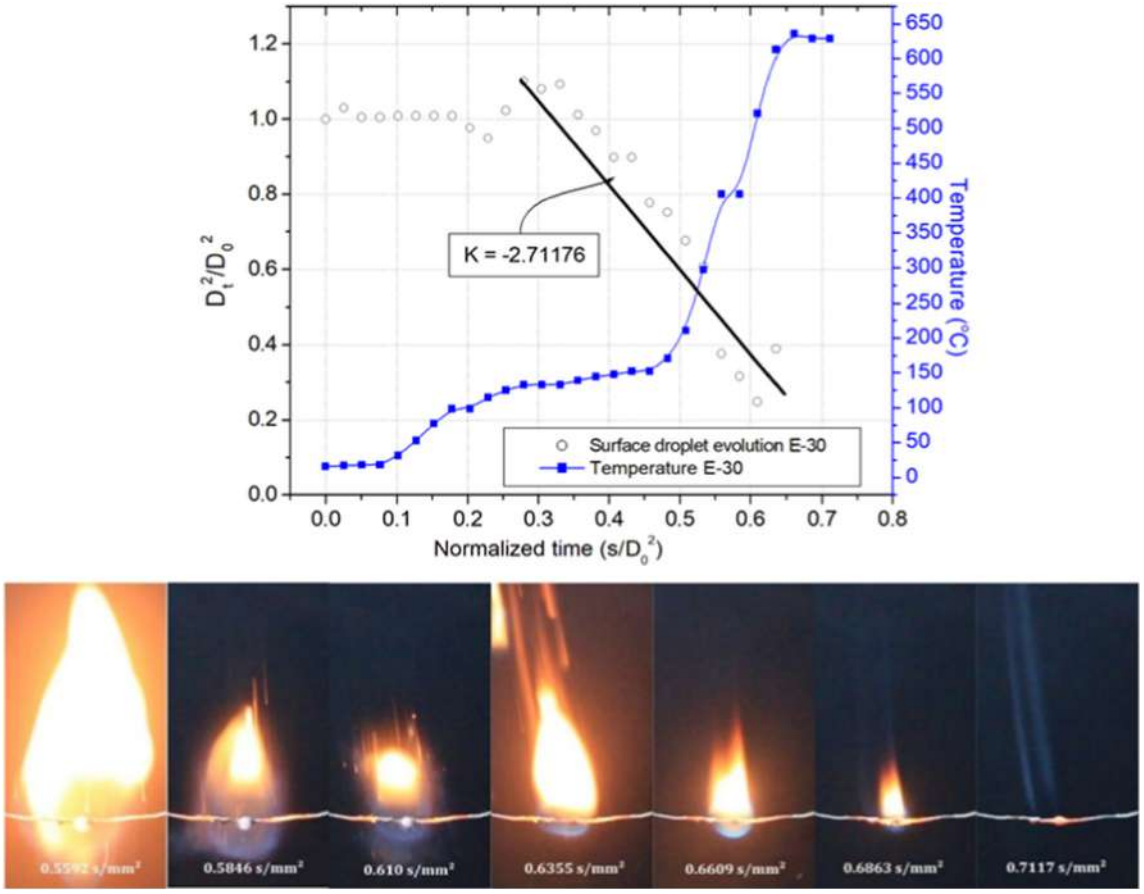

Fig. 7. Single droplet combustion of 30% v/v fraction mixture.

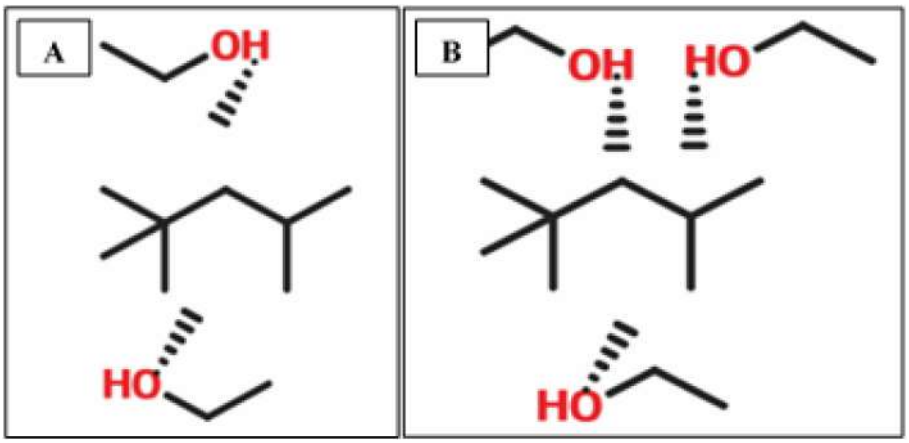

Fig. 8. Molecule model of ethanol iso-octane cluster, A: 41.4810% v/v; B: 51.5332% v/v.

than the others. However, from Figs. 2 and 3, it can be seen that the micro-explosion of droplet ethanol fraction 15% v/v is less than the ethanol fraction 10% v/v. This is due to the error of 10% v/v ethanol fraction in forming molecular clusters > 15% v/v ethanol fraction (Table 2).

The 26.1678 v/v ethanol fraction (Fig. 4C) shows that one molecule of ethanol in its hydroxyl group induces one iso-octane molecule. Molecular interaction force in the mixture fraction of 26.1678% v/v is greater than the ethanol fraction of 10.5658% and 15.0535% v/v, because the partial charge of ethanol induces more iso-octane partial charge so that it produces a greater interaction force. However, a fraction of 25% v/v (Fig. 5) has a greater error in forming molecular clusters, which is equal to 1.16783% v/v (Table 2), so that the intensity of micro-explosion in droplets is higher. Fig. 5 also shows that at the initial stage of combustion only a small amount of puffing droplet occurs until about 0.2 normalized time. This phenomenon indicates that molecular cluster interaction forces are stronger than ethanol fractions of 10% and 15% v/v.

From the description of the discussion of ethanol fraction up to 25% v/v (low levels) related to molecular interaction forces confirm that polar ethanol can induce non-polar iso-octane (hydrocarbons) and tend to form cluster of molecules which change the physical properties of each mixture form. However, detailed observations in this study provide slightly different findings of molecular cluster than previously

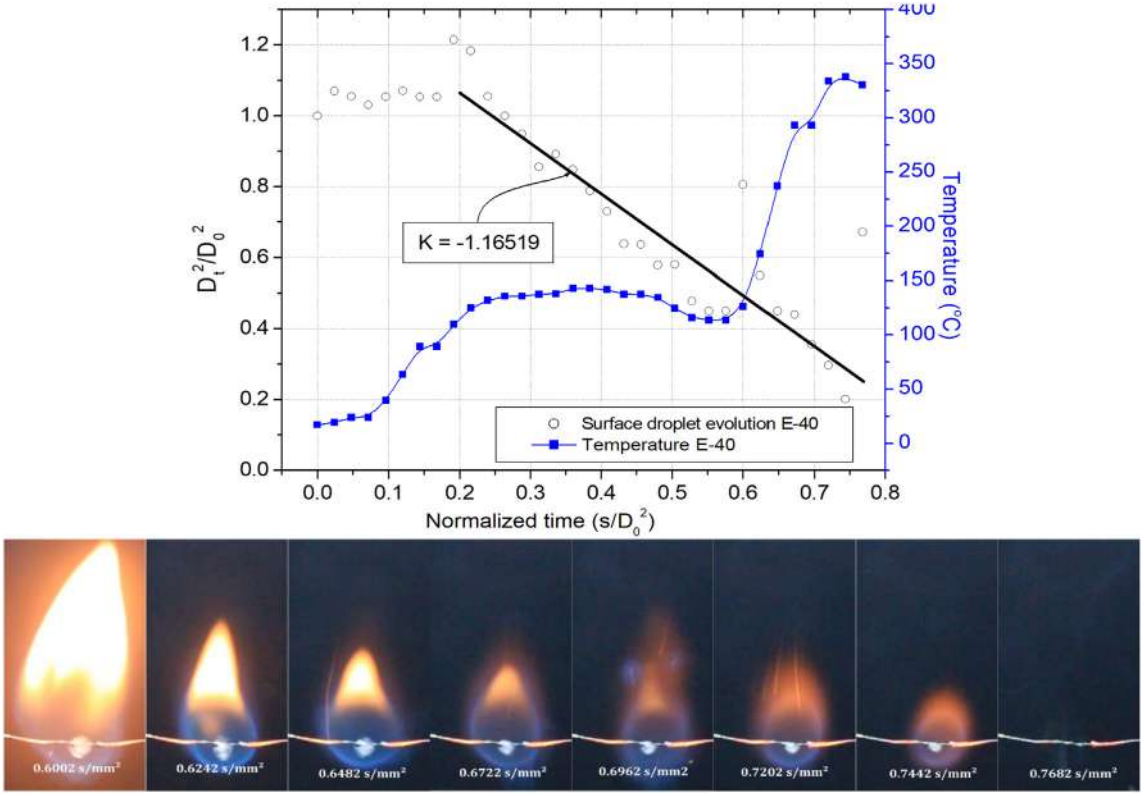

Fig. 9. Single droplet combustion of 40% v/v fraction mixture.

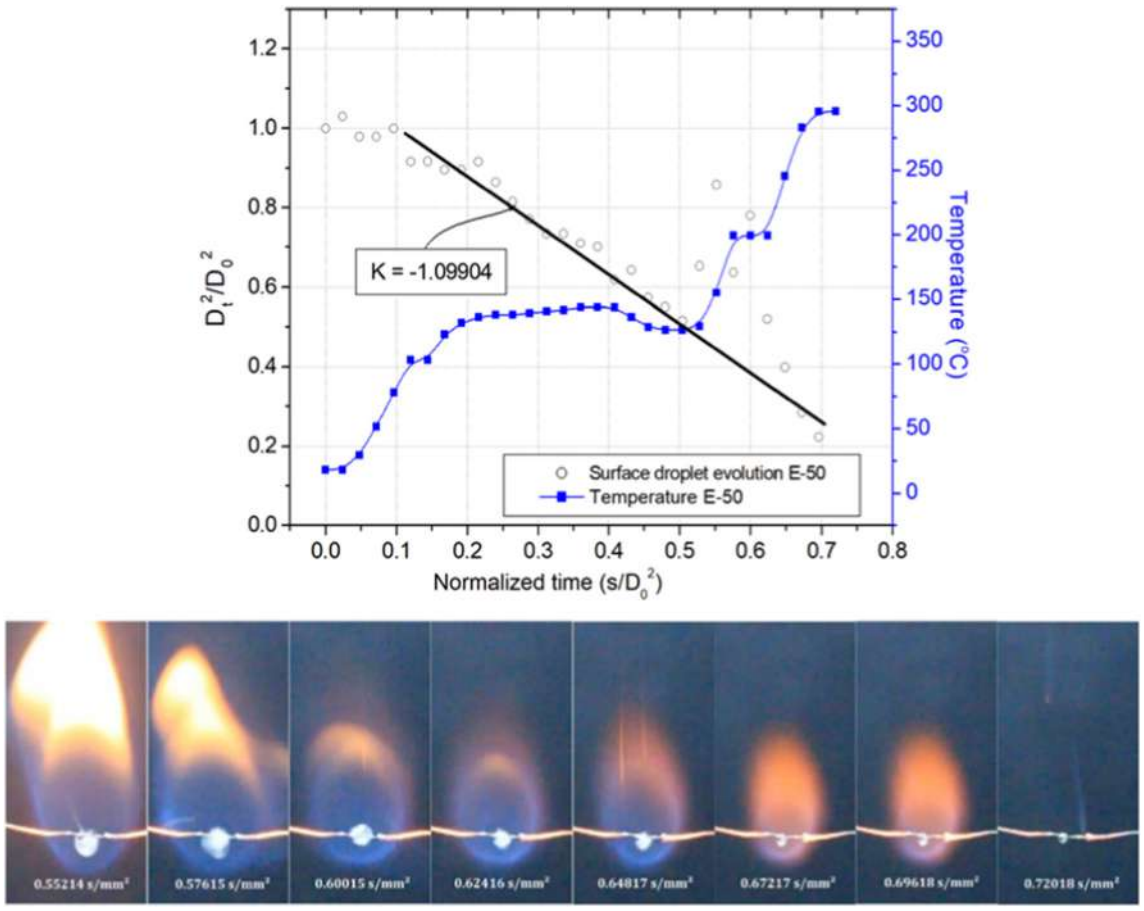

Fig. 10. Single droplet combustion of 50% v/v fraction mixture.

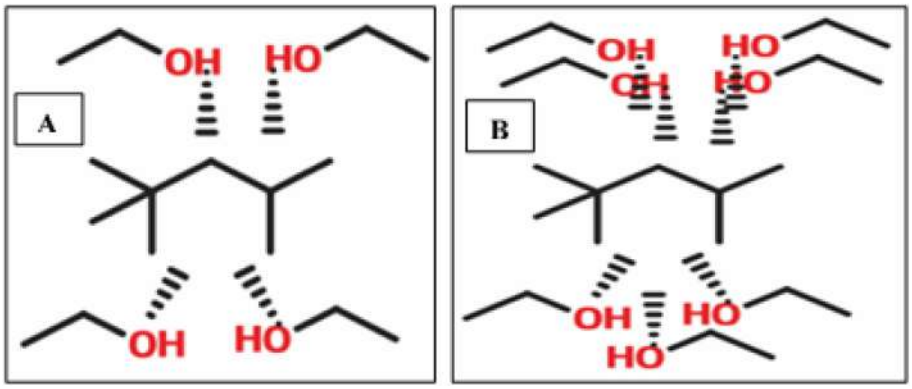

Fig. 11. Molecule model of ethanol iso-octane cluster, A: 58.6382% v/v; B: 71.2723% % v/v.

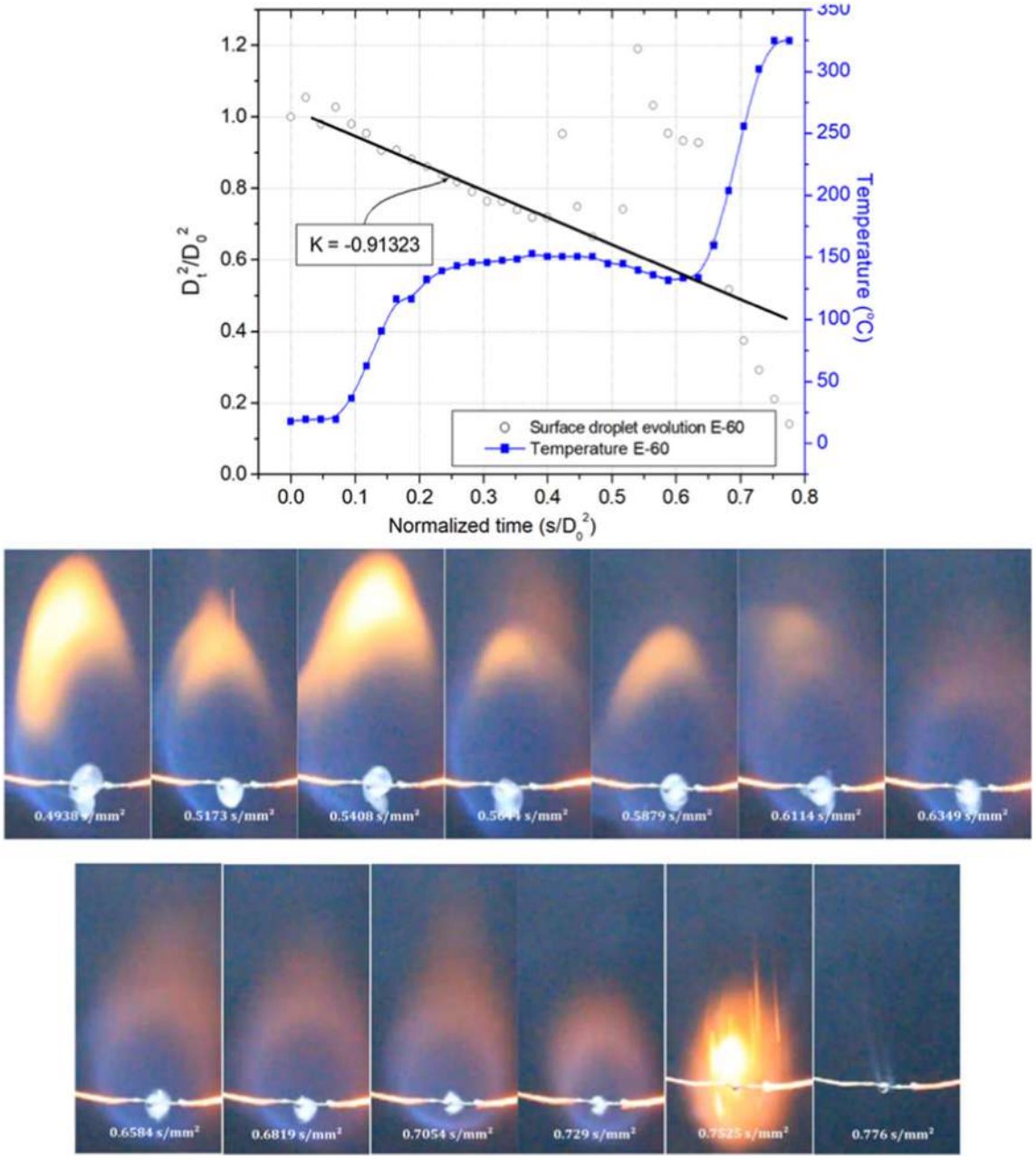

Fig. 12. Single droplet combustion of 60% v/v fraction mixture.

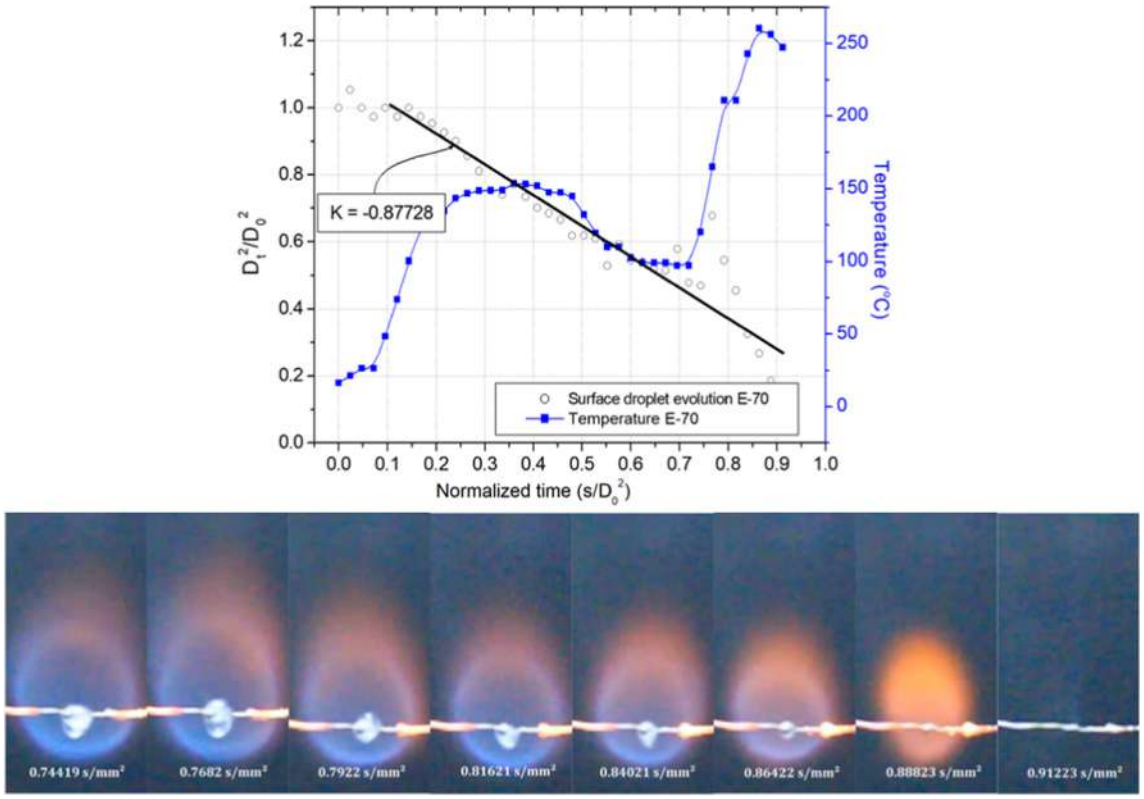

Fig. 13. Single droplet combustion of 70% v/v ethanol fraction.

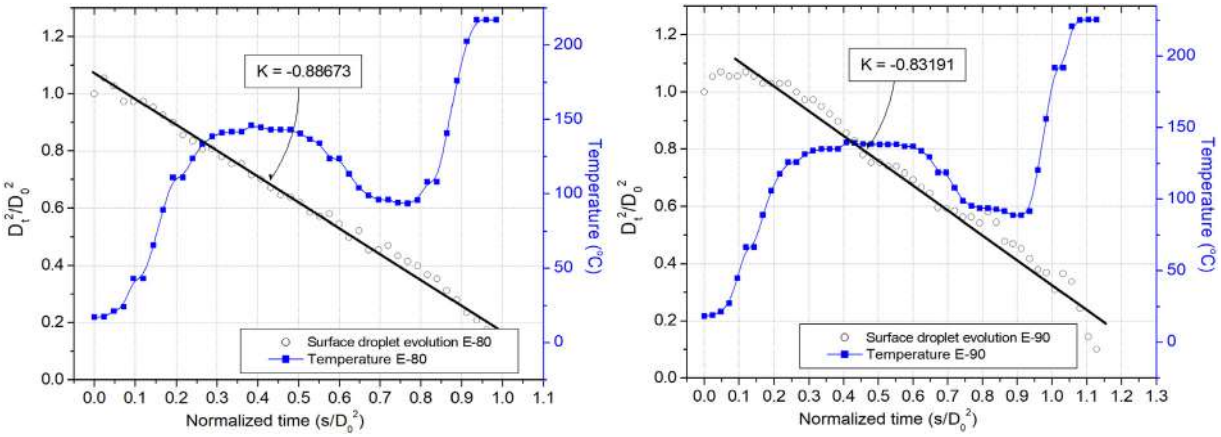

Fig. 14. Single droplet combustion of 80% and 90% v/v ethanol fraction ethanol fraction.

reported that molecular cluster is formed only in the fraction of the mixture of ethanol 41, 48% v/v [22]. The formation of molecular groups in this study is closer to the application of real combustion compared to the methods carried out previously [17].

The 20% and 30% v/v ethanol fractions are the fuel mixture fractions which are not adjacent to the mixture fraction which has the potential to form clustered molecules. Figs. 6 and 7 show that in the initial stage of combustion, puffing droplets regime occur up to 0.35 units of normalized time. In the mixture fraction of 20% and 30% v/v, a small cluster of molecules is formed which has a low boiling point, and more molecules are formed free of ethanol or iso-octane which have a higher boiling point. This little molecular cluster in the mixture fraction of 20% and 30% v/v produces lower total interaction force of molecules, so this results in a longer puffing droplet regime (0.35 unit of normalized time).

In the final stage, the combustion of droplets mixed with 20% ethanol and 30% v/v fractions resulted in a higher micro-explosive intensity than the mixed fractions of 10%, 15%, and 25% v/v (Figs. 6 and 7). This higher micro-explosion intensity results in a shorter combustion time with a higher constant burning rate (K = −2.72489 and K = −2.71126). However, Figs. 6 and 7 also show that the 30% v/v ethanol fraction has a higher micro-explosion intensity than the 20% v/v fraction. This phenomenon confirms the statement that the number of free molecules (unbound in molecular clusters) is more likely to produce an increasingly high-intensity of micro-explosions.

Figs. 9 and 10 are blends with ethanol fraction of 40% and 50% v/v with error cluster fractions of 1.48099% and 1.53323%, respectively (Table 2). The model of molecular interaction approach in this fraction is presented in Fig. 8 below,

Fig. 8A and B describe that one iso-octane molecule is induced by two and three iso-octane molecules in each cluster molecule formed so that the ethanol fraction cluster molecules Fig. 8B (51.5332% v/v) has a

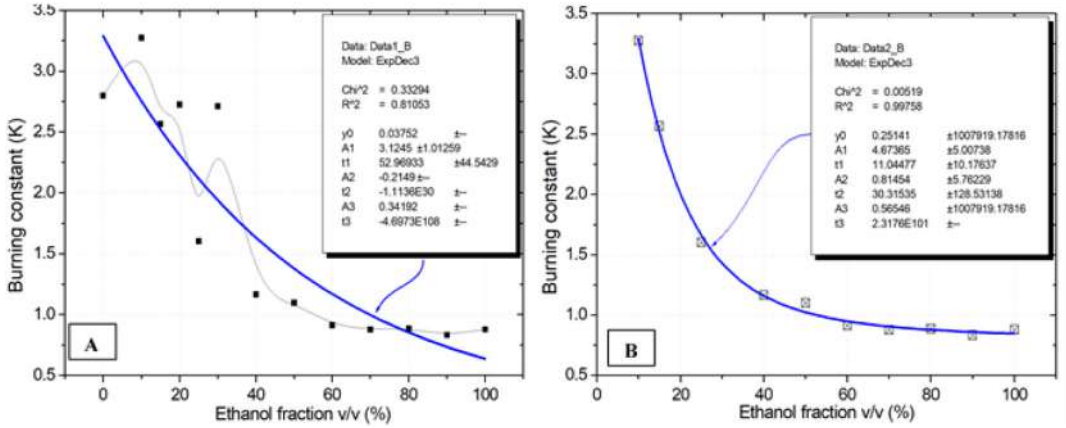

Fig. 15. Burning rate constant (K) for; A. All of ethanol iso-octane fraction, B. Without 20% and 30% v/v ethanol fraction.

sum of molecular interaction force greater than the lower ethanol fraction. While Figs. 9 and 10 show the puffing droplet of this mixture fraction, each occurs up to about 0.15 and 0.10 normalized unit time. This fact confirms the change in physical properties of the mixture that the higher the number of molecular interaction forces in the molecular cluster tends to cause the lower puffing droplet at the initial stage of combustion of droplets.

Single droplet combustion for higher ethanol fractions are shown in Figs. 12 and 13. In the high ethanol fraction, fuel blend has the potential to form larger molecular clusters because it involves more molecular journals. Molecular cluster modeling for ethanol fractions of 58.6382% and 71.2723% v/v are presented in Fig. 11 below,

Fig. 11A and B shows that in the ethanol fraction of 58.6382% and 71.2723% v/v, one iso-octane molecule is each induced by four and seven ethanol molecules. Sum of molecular interaction forces in each molecular cluster for higher ethanol fractions are also higher. However, for ethanol fraction of 58.6382% v/v is more stable because it has a more balanced partial polarity on both sides.

Figs. 12 and 13 show that at 60% and 70% ethanol fractions (high fraction), there is sort puffing droplet regime at the first stage of the single droplet burning. However, at the final stage, tend to produced a high-intensity micro-explosion. This phenomenon occurs because 60% and 70% v/v ethanol fraction have a large molecular cluster formation error of 1.36175% and 1.27231% v/v, respectively (Table 2). The increasing fraction of ethanol tend produces a huge molecular cluster and resulting in a higher boiling point difference between molecular clusters and iso-octane. The results of this study are in line with Wardana statement, which states that large boiling point differences tend to produce micro-explosion phenomena in single droplet combustion [32]. However, at high fractions droplets have lower LHV, so the droplet evaporation rate is also lower. The burning rate constant (K) correlates with the speed of evaporation and the intensity of the micro-combustion of the fuel blend droplet.

Fig. 14 describes the evolution of the droplet area during combustion along the high fraction ethanol mixture (80% and 90% v/v). This high fraction produces large molecular clusters because one iso-octane molecule is induced by many ethanol molecules (Table 2) so that the number of molecular clusters of high fraction molecular interaction forces is also large. Fig. 14 also confirms that at the initial stage the puffing droplet tends to occur slightly. Table 2 provides information that the error of molecular clusters in the ethanol fraction is 80%, and 90% which is very small, i.e. respectively 0.96354% and 0.21048% v/v. This small molecular cluster error produces smooth burning without micro-explosion during single droplet combustion.

3.3. The burning rate constant of various fractions of ethanol iso-octane blends

The burning rate is estimated from d^2 law, $k = d(d^2)/dt$ [33]. The results are presented in Fig. 15 as burning rate constant (K) versus various ethanol iso-octane fraction.

Fig. 15A shows the trend line of the burning rate constant (K) in various mixed fractions, including fractions of 20% and 30% v/v, which are considered to have no closeness to the composition of the mixture that forms a molecular group (Table 2). Fig. 15B is a burning rate constant (K) in various blends that are close to the composition of the mixture that forms a group of molecules. Fig. 15A and B show that increasing the ethanol fraction tends to reduce the rate of droplet burning. Increasing ethanol fraction tends to increase the geometry of molecular groups and the total intermolecular forces (Figs. 4, 8 and 11), thereby reducing the intensity of micro-combustion (Figs. 13 and 14). The increase in ethanol fraction also tends to increase the total latent heat of evaporation droplets (Table 1); the rate of evaporation decreases. The evaporation rate correlates with droplet burning rate constant (K) [34].

Fig. 15 confirms that the initial hypothesis that polar ethanol molecules tend to induce non-polar iso-octane molecules (hydrocarbons) and have the potential to form molecular groups that change the physical properties of each constituent molecule (ethanol and iso-octane). Although molecular interactions do not produce different chemical properties, changes in the physical properties of the iso-octane ethanol blend have been shown to determine the speed of chemical reactions during single droplet combustion.

4. Conclusions

Calculation of mole analysis was carried out to predict the composition of the mixture which has the potential to form molecular clusters. Single droplet combustion was carried out to prove the role of polar ethanol in inducing non-polar iso-octane empirically. Puffing and micro-explosion phenomena during the droplet combustion process explain the concept of the interaction of ethanol and iso-octane molecules. So that the role of molecular interactions of various iso-octane ethanol blends on the burning rate constant can be explained comprehensively. An important conclusion of this research is as follows,

a. The duration and intensity of puffing droplets during single droplet combustion of polar ethanol mixtures with non-polar iso-octane is influenced by the total force of molecular interactions in the formed molecular clusters.
b. The number of free molecules that do not form molecular clusters tends to produce micro-explosions at the final stage of single droplet

combustion.

c. Increasing ethanol fractions in molecular clusters tends to reduce the combustion rate constant exponentially.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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