



## Full Length Article

## The role of ethanol as a cosolvent for isooctane-methanol blend

Budi Waluyo<sup>a</sup>, Muji Setiyo<sup>a,\*</sup>, Saifudin<sup>a</sup>, I.N.G. Wardana<sup>b</sup><sup>a</sup> Department of Automotive Engineering, Universitas Muhammadiyah Magelang, 56172, Indonesia<sup>b</sup> Department of Mechanical Engineering, University of Brawijaya, Malang 65141, Indonesia

## ARTICLE INFO

## Keywords:

Isooctane-methanol blend  
Ethanol  
Cosolvent

## ABSTRACT

Methanol has a strong potential to be used as a substitution for fossil fuel due to its several advantages such as the enthalpy of evaporation, high octane numbers and high oxygen content. However, unlike the non-polar gasoline, it is polar and very miscible with water and this leads to the phase separation of the gasoline-methanol blend. Therefore, this study was conducted to understand the role of ethanol in improving the homogeneity and stability of the gasoline-methanol blend. Molecular analysis was conducted through the HyperChem software to simulate important molecular properties of each constituent substance. Isooctane as a single substance was chosen to represent multi-substance gasoline to simplify the analysis of molecular interactions. Experimental tests were also conducted by mixing several fractions of the isooctane-methanol blend, and the ethanol was dripped gradually into separate phases of the mixture. The manual stirring was conducted, then allowed to stay for 120 s on each drop. Visual observation and addition of ethanol drops were stopped after the mixture separation phase did not occur. The results showed a certain amount of ethanol (up to 22%) was needed to improve the homogeneity and stability of the isooctane-methanol blend. The ethanol fractions up to 22% v/v needs to be added to block hydrogen bonds between the methanol-water molecules. The addition of ethanol produces new hydrogen bonds that were stronger than the methanol and water bond to improve the homogeneity and stability of the isooctane-methanol blend.

## 1. Introduction

The depletion of fossil fuel reserves and the deterioration of the environment due to greenhouse effect makes the investigation on the use of alcohol in spark-ignition engines (SI engines) become a focus of sustainable energy research [1]. Several previous studies conducted showed that alcohol produced lower emissions and has good performance [2]. Moreover, methanol and ethanol are the most potential biofuels to be used as substitutes for gasoline without significant changes in engine structure [3,4]. This has attracted the attention of previous researchers because of their ability to be produced from renewable energy sources and their oxygen content which enables complete combustion [5]. Methanol and ethanol are the leading candidates to replace conventional SI Engine fuels due to some of their physical properties and the similarity in combustion compared to gasoline. The other advantages include high octane numbers, good stoichiometric flame speeds, high octane sensitivity, and high heat evaporation [6,7].

Furthermore, scalability is one of the reasons some researchers have developed methanol as an SI Engine fuel. The ease of being produced from several raw materials makes it a strong alternative for sustainable fuels towards reducing the effects of carbon dioxide from transport

activities [8]. Methanol has also been successfully applied to diesel engines through a new combustion scheme which involves gas phase by forming a homogeneous mixture in the combustion chamber (diesel-methanol dual-fuel/DMDf combustion). Methanol with diesel fuel can operate stably up to a fraction of 30% in practical use [9].

Methanol also has a higher enthalpy of evaporations than ethanol, therefore, it has the potential to produce lower NO<sub>x</sub> emissions [10]. It can be produced by first converting almost all biomass to synthesis gas in a gasifier, from carbon dioxide and water or water vapor [11]. It can also be produced from carbon dioxide or hydrogen by using renewable energy and other energy sources [12]. Methanol is the simplest molecules of the alcohol group and has many similarities with ethanol in physical and combustion properties [8]. Its use in SI engine is also expected to increase the thermal efficiency of combustion [13]. Another advantage of using methanol as a sustainable fuel is the lower boiling point, more oxygen content, and higher evaporation pressure compared to ethanol [14]. However, it has several disadvantages such as cold start problems and lower energy density than ethanol, thus limiting its practical application in SI engine [15]. It is also a hydrophilic liquid with the ability to cause problems when transported through pipes [16].

\* Corresponding author.

E-mail address: [setiyo.muji@ummgl.ac.id](mailto:setiyo.muji@ummgl.ac.id) (M. Setiyo).<https://doi.org/10.1016/j.fuel.2019.116465>

Received 19 August 2019; Received in revised form 17 October 2019; Accepted 20 October 2019

Available online 06 November 2019

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The main problem with the methanol-gasoline blend as SI engine fuel is phase separation at low temperatures [11]. The separation of the mixture depends on the composition of the base gasoline, the percentage of methanol, and the water content [17]. Moreover, the homogeneity of the liquid phase of the blend is also very unstable, leading to new problems in its use. The phase separation of methanol gasoline blend is caused by the polarity of the compound which makes it very soluble in water, unlike the non-polar gasoline which cannot be mixed with water. The solubility of ethanol in gasoline is better than methanol and this makes ethanol to be suitable as a cosolvent of the blend [18]. However, up to now, there is no satisfactory explanation for the differences in the solubility of methanol and ethanol from gasoline even though they are both simple chain alcohol.

This study disclosed the differences in the solubility of methanol and ethanol with gasoline based on the analysis of the molecular interactions. The physical properties were determined by interactions between molecules which are also influenced by the geometry and the partial charge of each of its constituents. Isooctane was chosen as a single substance to represent gasoline [19] to simplify the analysis due to the multi-substance nature of gasoline. Moreover, molecular interaction simulation was conducted using HyperChem software to calculate the atomic partial charge and geometry of each molecule constituent.

## 2. Experimental setup

### 2.1. Fuel blends preparation

Isooctane (2,2,4-trimethylpentane) was used for analysis (CAS-No: 540-84-1) to represent gasoline as a fossil fuel. It was supplied as a single substance by Merck, Germany. Methanol (methyl alcohol) was a liquid with the formula  $\text{CH}_3\text{OH}$  having a level of 99.8% in this study (CAS-No. 67-56-1). Isooctane and methanol had molecular weights of 114.23 and 32.04  $\text{g}\cdot\text{mol}^{-1}$ , respectively.

Ethanol (ethyl alcohol) used as the cosolvent to improve the homogeneity and stability of isooctane methanol fuel blend was the analytical reagent grade (CAS-No: 64-17-5) supplied by the Indonesian Smart-lab. The detailed properties of the fuel are presented in Table 1.

Furthermore, this study used a fraction blend of isooctane methanol 95%, 90% up to 0% v/v, with a total volume of the mix being 5 ml. The mixing process was conducted manually in a closed reaction glass. At room temperature, the isooctane-methanol fuel blend was separated into several fractions of mixtures as shown in Fig. 1.

### 2.2. Fuel molecular modelling

This was conducted to identify the essential parameters of each constituent fuel through the use of Hyper Chem release 8.0.10 under

**Table 1**  
Properties of test fuels.

Properties	Isooctane	Methanol	Ethanol
Purity (%)	99.5	99.8	99.7
Chemical formula	$\text{C}_8\text{H}_{18}$	$\text{CH}_3\text{OH}$	$\text{C}_2\text{H}_5\text{OH}$
Boiling Temperature ( $^{\circ}\text{C}$ )	98–100	64.6	78.3 [20]
Flash point ( $^{\circ}\text{C}$ )	–12	11	13
Enthalpy of evaporations at 25 $^{\circ}\text{C}$ ( $\text{kJ}\cdot\text{kg}^{-1}$ ) [21]	308	1178 [22]	924.2
H/C ratio	2.25	4	3
Low heating value ( $\text{MJ}\cdot\text{kg}^{-1}$ )	44.4	19.7 [22]	26.83
Molecular Weight ( $\text{g}\cdot\text{mol}^{-1}$ )	114.23	32.04	46.07
Density @ 20 $^{\circ}\text{C}$ ( $\text{g}\cdot\text{cm}^{-3}$ )	691.9	792	789
Acidity (%)	0.0003	0.001	0.0006
Vapor pressure at 20 $^{\circ}\text{C}$ (kPa)[23]	5.5	13.02	5.95
Oxygen content (wt%) [23]	0	49.93	34.73
Solubility in water	Insoluble	Soluble	Soluble

windows version for simulation. Hydrogen bonding between polar ethanol and methanol and molecular interactions with non-polar isooctane were simulated by the semi empirical quantum mechanical method also provided by HyperChem. Moreover, the CNDO method was used to calculate electronic properties at the optimum geometry conditions of each fuel constituent.

### 2.3. Experimental apparatus

This was used to obtain the minimum ethanol requirements needed to form a fossil-alcohol fuel mixture without separation at several fractions blended which were mixed manually in closed reaction glasses as shown in Fig. 2. Moreover, a DSLR camera was placed 50 cm in front of the reaction glass while two back-light was set to the right and left to obtain optimum image results as shown in Fig. 2.

This experiment was conducted at a temperature and pressure of 25  $^{\circ}\text{C}$  and 1 atm respectively, while the humidity was conditioned between 50%–55%. The ethanol and methanol tubes were always closed with a rubber cap to minimize the ingress of water vapor from the air and allow syringe needle to pass through.

Moreover, 0.5 ml drop of the cosolvent ethanol was added to the fuel blend using a 1 ml syringe and manually stirred every time. Visual observation was conducted at a waiting period of 60 s in each pot-stirring of the fuel fraction blend. Snapshots of several fractions were taken with DSLR cameras after the homogeneous mixture was formed.

## 3. Result and discussion

### 3.1. The atomic partial charge of the constituents

The atomic partial charge determines the magnitude of the intermolecular force (IMF) and influences the molecular electrostatic interaction energy. Moreover, intermolecular force defines the force of attraction or repulsion between the molecules and other neighboring particles and this affects the homogeneity of two or more substances blends. The partial atomic charge of isooctane and methanol obtained with the HyperChem software are presented in Tables 2 and 3.

Tables 2 and 3 show isooctane has an atomic partial charge distribution of less than 0.1 e and this value is spread evenly across all its atoms. This small difference makes it a non-polar covalent bonding group [24]. However, methanol molecule with hydroxyl (OH) groups have a partial charge difference of 0.559 e ( $> 0.5$  e) between O and H atoms (2 and 6) making it a polar covalent group. While the partial charge for ethanol molecules obtained from the HyperChem software is presented in Table 4.

Ethanol is an alcohol group with two carbon atoms and a hydroxyl group (OH). The difference in the partial charge of the O and H atoms in the hydroxyl group (3 and 9) was 0.597 e ( $> 0.5$  e), which classifies it as a polar covalent group. The difference in the partial charge on the hydroxyl of methanol is higher than ethanol, therefore, methanol has a stronger intermolecular force on the hydroxyl group.

However, ethanol has a longer carbon chain (C2) than methanol (C1), and this makes it has a more molecular surface area. The simulation results and the calculation of the molecule surface area of methanol and ethanol are presented in Figs. 3 and 4.

The surface area also affects molecular interactions because it determines and directly proportional to the surface tension between molecules.

### 3.2. Molecular interactions simulation between fuel constituents

The molecular interactions between the constituents determined the solubility of one substance in another. The blending of non-polar isooctane with polar methanol tends to separate in almost all mixed fractions (Fig. 1). The separation of polar methanol and non-polar isooctane is due to methanol is effortless to form hydrogen bonds with

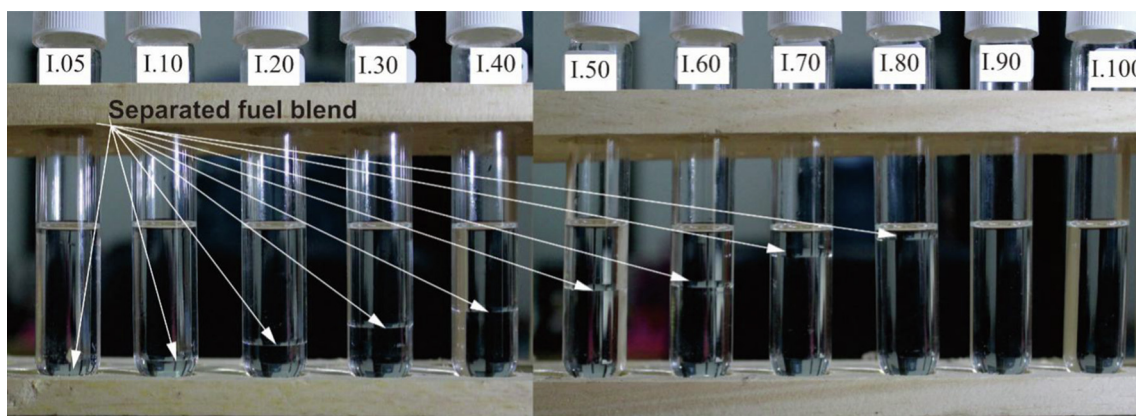


Fig. 1. Separated isooctane-methanol fuel blend.

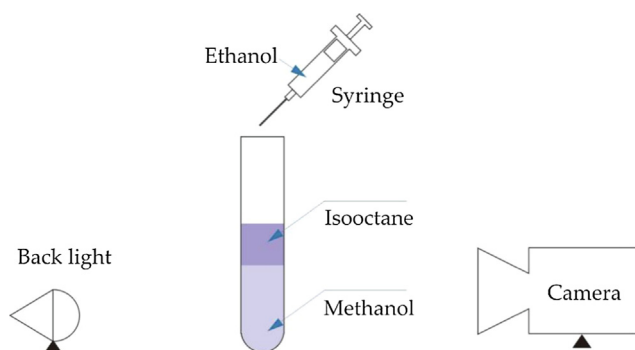


Fig. 2. The experimental setup apparatus.

Table 2  
The atomic charge of isooctane.

No	Symbol	Partial Charge	
Atom 1.	C	-0.063 e	
Atom 2.	C	-0.e	
Atom 3.	C	-0.038 e	
Atom 4.	C	-0.060 e	
Atom 5.	C	-0.060 e	
Atom 6.	C	-0.046 e	
Atom 7.	C	-0.047 e	
Atom 8.	C	-0.063 e	
Atom 9.	H		0.023 e
Atom 10.	H		0.023 e
Atom 11.	H		0.023 e
Atom 12.	H		0.024 e
Atom 13.	H		0.024 e
Atom 14.	H		0.024 e
Atom 15.	H		0.024 e
Atom 16.	H		0.024 e
Atom 17.	H		0.024 e
Atom 18.	H		0.024 e
Atom 19.	H		0.024 e
Net Charge		-0.395 e	0.395 e

Table 3  
The atomic charge of methanol.

No	Symbol	Partial Charge	
Atom 1.	C		0.033 e
Atom 2.	O	-0.395 e	
Atom 3.	H		0.052 e
Atom 4.	H		0.052 e
Atom 5.	H		0.052 e
Atom 6.	H		0.204 e
Net Charge		-0.395 e	0.395 e

Table 4  
The atomic charge of ethanol.

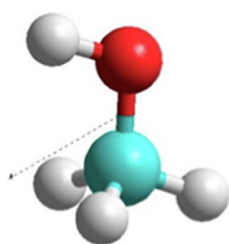
No	Symbol	Partial Charge	
Atom 1.	C	-0.042 e	
Atom 2.	C		0.041 e
Atom 3.	O	-0.392 e	
Atom 4.	H		0.025 e
Atom 5.	H		0.025 e
Atom 6.	H		0.025 e
Atom 7.	H		0.056 e
Atom 8.	H		0.056 e
Atom 9.	H		0.205 e
Net Charge		-0.434 e	0.434 e

water so that the critical phase separation temperature (CPST) of the blend increases [17,18]. The results obtained using HyperChem software semi empirical quantum mechanical methods are presented in Fig. 5. However, the dipole moment of isooctane methanol molecular interactions are presented in Table 5.

Methanol and ethanol are short-chain alkane with hydroxyl (OH) at one end making both of them polar. The partial charge of their hydroxides has the potential for quite interesting molecular interactions like hydrogen bonds to pull together. The initial temperature of the simulations set at room temperature (300 K). Ethanol-methanol molecular cluster simulation with hydrogen bonds tends to produce slower random movements than methanol so, the final temperature was lower (273.20 K). Meanwhile, simulation of polar methanol and non-polar isooctane, random motion of polar methanol molecules was faster so that the final temperature of the blend is higher (360.76 K). HyperChem simulation results show that there is an attraction between the oxygen atom in the methanol hydroxyl group and the hydrogen atom in the hydroxyl ethanol group to form a hydrogen bond (Fig. 6). This bonding ensures a higher boiling point for methanol and ethanol than alkane groups without hydroxyl (OH). The results for methanol and ethanol are shown in Fig. 6.

Meanwhile, the addition of ethanol to the isooctane methanol blend tends to improve molecular interactions between its constituents. Methanol-ethanol molecular interactions tend to form molecular clusters so that they are like single substances. The molecular clusters of methanol-ethanol have a larger surface area so that the total surface tension increases, that's resulting in a stronger interaction style with non-polar isooctane. The results for an isooctane-methanol-ethanol blend using HyperChem software are presented in Fig. 7 as follows.

The interaction of methanol and ethanol molecules through hydrogen bonds has a more intermolecular force and a tendency to form molecular clusters [25]. This also leads to a new geometry in interacting with isooctane molecules. However, the cluster of the methanol-ethanol molecule was observed to have a larger surface area with



Atom 1	C	21.558 Å <sup>2</sup>
Atom 2	O	29.028 Å <sup>2</sup>
Atom 3	H	25.062 Å <sup>2</sup>
Atom 4	H	25.466 Å <sup>2</sup>
Atom 5	H	26.544 Å <sup>2</sup>
Atom 6	H	30.586 Å <sup>2</sup>
Methanol net surface area		158.243 Å <sup>2</sup>

Fig. 3. Molecule surface area of methanol.

265,950 Å<sup>2</sup> and this determines the surface tension required to increase the intermolecular force of the blend. Moreover, the dipole moment of isooctane-methanol molecular interactions are presented in Table 6.

The molecular interaction simulation results with HyperChem software also showed the addition of ethanol to the isooctane-methanol blend has the ability to improve molecular interactions among its constituents. This is shown in the increasing total dipole moment of the blend with 1806 debyes obtained for isooctane-methanol as shown in Table 5 and 3,840 debyes for isooctane-methanol-ethanol as shown in Table 6.

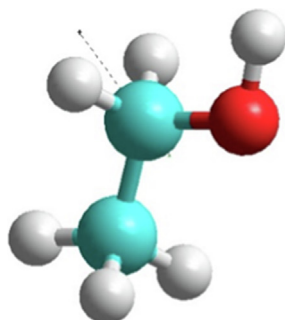
### 3.3. Ethanol as a cosolvent of isooctane-methanol blend

This test was conducted to determine the minimum ethanol requirements to be added to the isooctane-methanol blend to produce an inseparable fuel mixture. The mixture at several fractions of I.05, I.10, I.20, up to I.100 was stirred manually and waited for 120 s. The results revealed the blend was separated in all mixed fractions as shown in Fig. 1. Furthermore, Table 7 shows the results of adding ethanol into the isooctane-methanol blend up to when there was no separation. The minimum ethanol required to improve the quality of the isooctane-methanol mixture in several mixed fractions as shown in Table 7.

The fuel column in Table 7 shows the fuel mixture fraction I. yy which means the mixture consists of 95% v/v isooctane and 5% methanol as well as 5% fuel blend fraction for methanol. The addition of ethanol to the isooctane-methanol mixture at several mixed fractions was proven to produce a homogeneous fuel blend without separation. Moreover, the snapshot of the optimum isooctane-methanol-ethanol blend without separation is shown in Fig. 8.

Table 7 and Fig. 8 show that in the 90% v/v, methanol isooctane fraction (I.10) produced a homogeneous fuel blend without separation. This was due to the ability of polar methanol to induce polar isooctane in small quantities. The relationship between the ethanol-methanol ratios to several fractions of isooctane-methanol blend to produce a homogeneous mixture is presented in Fig. 9, that the ratio has a decreased linear tendency in line with the isooctane fraction.

Therefore, the addition of ethanol to the isooctane-methanol blend has the ability to change the configuration of the mixture fraction for each of its constituents to achieve a triangular relationship of isooctane-



Atom 1	C	14.271 Å <sup>2</sup>
Atom 2	C	5.567 Å <sup>2</sup>
Atom 3	O	24.550 Å <sup>2</sup>
Atom 4	H	24.118 Å <sup>2</sup>
Atom 5	H	23.916 Å <sup>2</sup>
Atom 6	H	24.388 Å <sup>2</sup>
Atom 7	H	23.445 Å <sup>2</sup>
Atom 8	H	23.647 Å <sup>2</sup>
Atom 9	H	30.384 Å <sup>2</sup>
Ethanol net surface area		194.285 Å <sup>2</sup>

Fig. 4. Molecule surface area of ethanol.

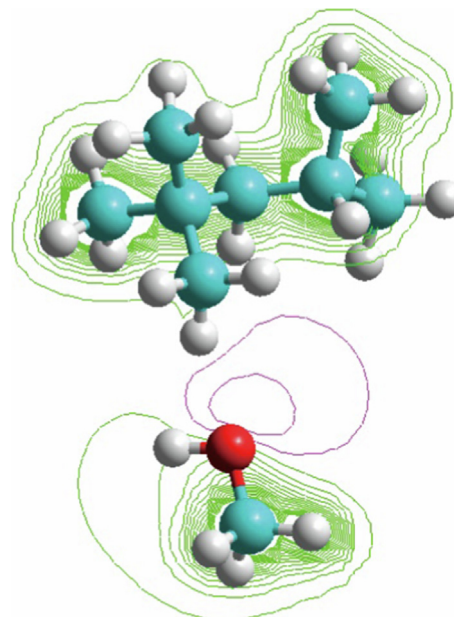


Fig. 5. Isooctane-methanol molecule interaction graphs.

methanol-ethanol fuel blend as shown in Fig. 10.

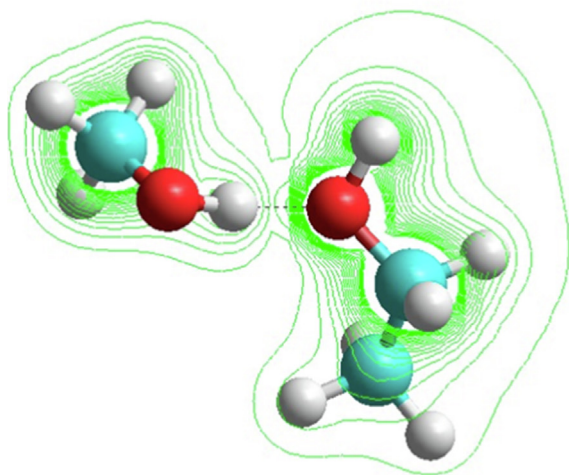
Furthermore, phase separation in the isooctane-methanol blend as shown in Fig. 1 occurred due to the solubility of methanol in water because of their polarity as well as the insolubility of isooctane because of its non-polar nature. However, the solubility of methanol in ethanol is stronger than water due to the hydrogen bonds between their molecular constituents as shown in Fig. 11. Moreover, the difference in partial charge between atoms in the hydrogen bond of the methanol-ethanol blend was higher than the methanol-water blend, which means methanol is more soluble in ethanol than water.

The new geometry cluster of methanol-ethanol molecules as shown in Fig. 7 is more stable and difficult to bind water molecules, thereby, making the biofuel-fossil fuels blend become more homogeneous and stable. This is in line with the findings of Qi et al., 2005 that the use of



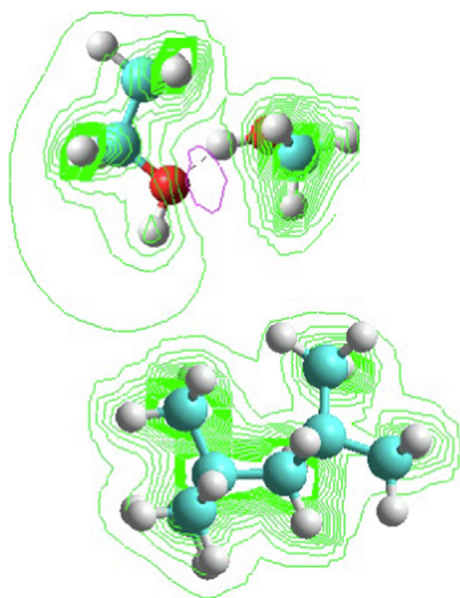
**Table 5**  
The dipole moment of isooctane-methanol molecule interaction.

Dipole (Debyes)	x	y	z	Total	
Point-Chg	0.612	0.156	-0.291	0.696	Time = 1.0000 ps
sp Hybrid	0.414	0.262	1.135	-1.236	Kinetic Energy = 34.4116 kcal/mol
pd Hybrid	0.000	0.000	0.000	0.000	Total Energy = -7444.8931 kcal/mol
Sum	1.026	0.418	-1.426	<b>1.806</b>	Temperature = 360.76 K (final)



Methanol		
Atom 1	C	21.861 Å <sup>2</sup>
Atom 2	O	23.191 Å <sup>2</sup>
Atom 2	H	14.956 Å <sup>2</sup>
Atom 2	H	23.108 Å <sup>2</sup>
Atom 2	H	25.398 Å <sup>2</sup>
Atom 2	H	3.032 Å <sup>2</sup>
Methanol net surface area		111.546 Å <sup>2</sup>
Ethanol		
Atom 1	C	14.169 Å <sup>2</sup>
Atom 2	C	7.287 Å <sup>2</sup>
Atom 3	O	6.158 Å <sup>2</sup>
Atom 4	H	17.247 Å <sup>2</sup>
Atom 5	H	23.714 Å <sup>2</sup>
Atom 6	H	10.577 Å <sup>2</sup>
Atom 7	H	22.973 Å <sup>2</sup>
Atom 8	H	22.704 Å <sup>2</sup>
Atom 9	H	29.575 Å <sup>2</sup>
Ethanol net surface area		154.404 Å <sup>2</sup>
<b>Total surface area</b>		<b>265.950 Å<sup>2</sup></b>

**Fig. 6.** Methanol ethanol molecule interaction surface area and graphs<sup>4</sup>.



**Fig. 7.** Molecular simulation results of an isooctane-methanol-ethanol blend.

**Table 6**  
The dipole moment of an isooctane-methanol-ethanol molecule interaction.

Dipole (Debyes)	x	y	z	Total	
Point-Chg	-1.060	0.831	-1.344	1.902	Time = 1.0000 ps
sp Hybrid	-0.629	1.077	-1.529	1.973	Kinetic Energy = 33.3882 kcal/mol
pd Hybrid	0.000	0.000	0.000	0.000	Total Energy = -9354.8364 kcal/mol
Sum	-1.689	1.907	-2.873	<b>3.840</b>	Temperature = 273.20 K (final)

ethanol as a cosolvent in the methanol-gasoline blend can resolve the problem of phase separation [18]. This was due to the ability of the methanol molecule to produce a stronger hydrogen bond with ethanol compared to water as revealed in Fig. 11 so that the mixture is able to block hydrogen bonds between the methanol-water molecules. Fig. 11 show that electronegativity difference between a mixture of methanol-ethanol and methanol-water. The higher the electronegativity difference, the stronger the molecular interaction force produced. This is in agreement with the statements of Osten, D.W and Sell, N. J, 1982 that stronger hydrogen bonds of alcohol groups tend to reduce the phase separation of the bio-fossil fuel blend [17]. The adding ethanol to the methanol-isooctane blend, some physical properties such as boiling point, vapor pressure, etc. will change. Changes in the physical properties of the fuel blends are caused by molecular interactions (hydrogen bonds) between ethanol and methanol (Fig. 11), so they tend to form molecular clusters [19].

#### 4. Conclusions

A certain amount of ethanol is required to improve the homogeneity and stability of the isooctane-methanol blend. This was simulated using HyperChem software and the result showed the simple and gradual dropping of ethanol into a separated phase isooctane-methanol blend has the ability to improve the mixture. The ratio of ethanol-methanol to several isooctane-methanol blend fractions showed a linear tendency to

**Table 7**  
The minimum requirement for ethanol to prevent the separation of the isooctane-methanol blend.

Fuel	Isooct. (mL)	Meth. (mL)	Ethanol (mL)															Total Eth (mL)	Total (I,M,E) (mL)	Eth. Frac. (%)	Meth. Frac. (%)	Isooct. Frac. (%)		
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15							
I.95	4.750	0.250	0.1	0.1	0.1															0.30	5.30	0.896	0.047	0.06
I.90	4.500	0.500	0.1	0.1	0.1	0.1	0.1	0.1												0.60	5.60	0.804	0.089	0.11
I.80	4.000	1.000	0.1	0.1	0.1	0.1	0.1	0.1	1.0	1.0	1.0	0.5							0.95	5.95	0.672	0.168	0.16	
I.70	3.500	1.500	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	1.40	6.40	0.547	0.234	0.22	
I.60	3.000	2.000	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	1.45	6.45	0.465	0.310	0.22	
I.50	2.500	2.500	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.05	1.35	6.35	0.394	0.394	0.21	
I.40	2.000	3.000	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.05		1.05	6.05	0.331	0.496	0.17	
I.30	1.500	3.500	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1							0.80	5.80	0.259	0.603	0.14	
I.20	1.000	4.000	0.1	0.1															0.20	5.20	0.192	0.769	0.04	
I.10	0.500	4.500																	0.00	5.00	0.100	0.900	0.00	
I.00	0.000	5.000																	0.00	5.00	0.000	1.000	0.00	

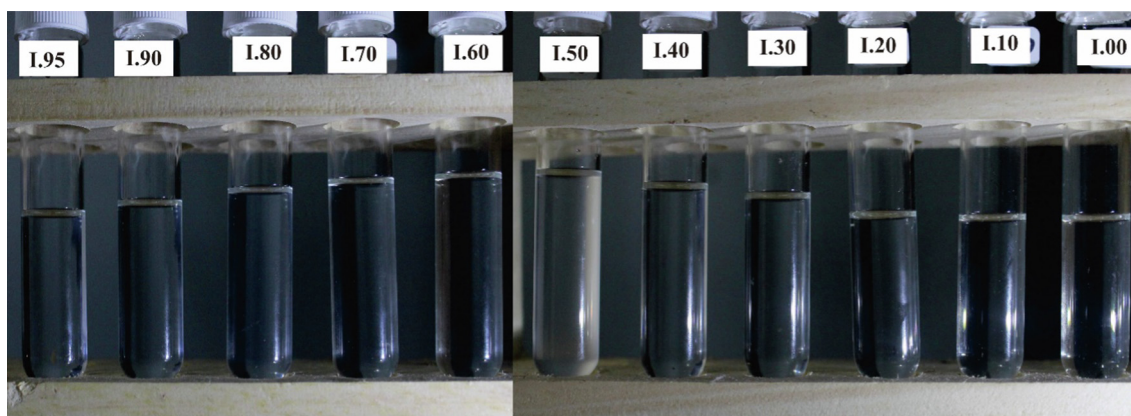


Fig. 8. The Isooctane-methanol-ethanol blend without separation.

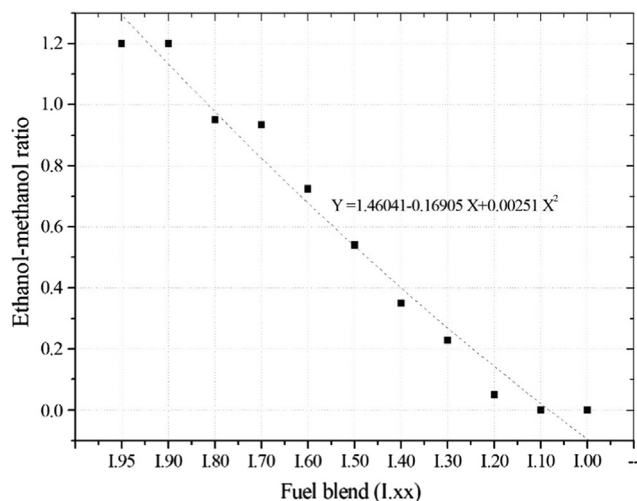


Fig. 9. The ethanol-methanol ratio blend to produce homogeneous fuel blend.

decrease in line with an increase in the methanol-isooctane fraction. The separation phase was caused by the miscibility of methanol with water due to their polarity and the difficulty in dissolving the isooctane due to its non-polar nature. The addition of other substances to produce stronger hydrogen bonds than methanol-water can improve the homogeneity and stability of the isooctane-methanol blend.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to

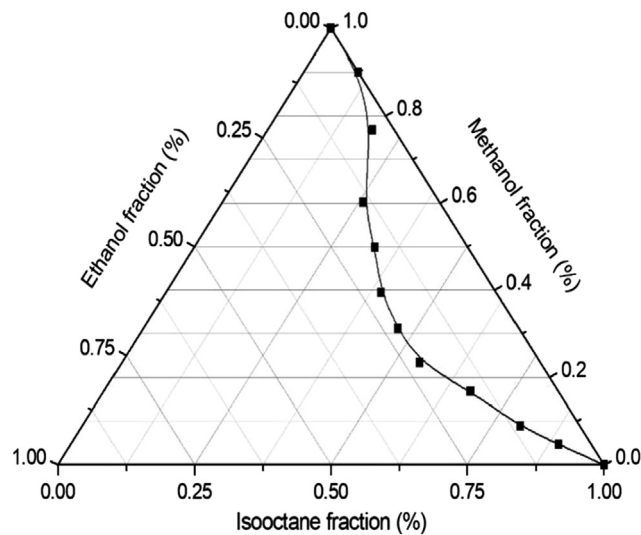


Fig. 10. Triangular relationship of the homogenous isooctane-methanol-ethanol blend.

influence the work reported in this paper.

**Acknowledgments**

The authors show gratitude to the Ministry of Research, Technology and the Higher Education, Republic of Indonesia for the grant provided for this research and the Automotive Laboratory, Department of Automotive, Universitas Muhammadiyah Magelang for supporting research materials.

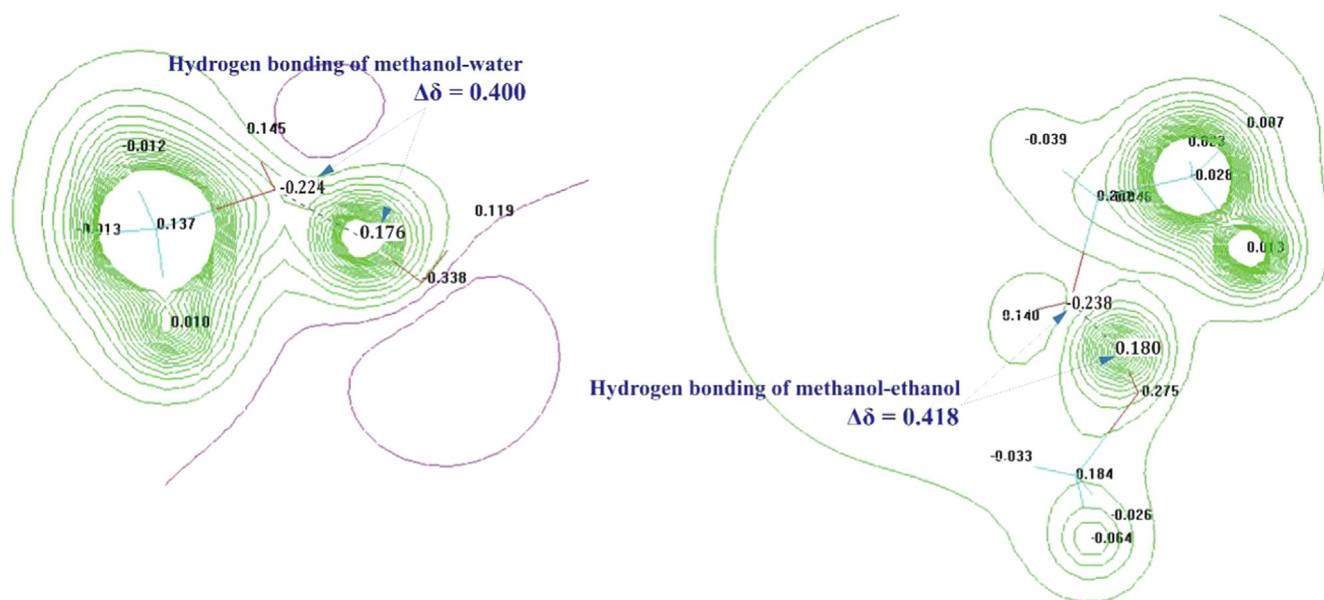


Fig. 11. Hydrogen bonding of methanol-water vs methanol-ethanol.

## Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fuel.2019.116465>.

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