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The Influence of Eugenol in Lubrication Properties of Crude Jatropha Curcas Lin

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Contact angle, molecular interaction, lubrication, vegetable oil, properties

Abstract

In machining processes, vegetable oil based lubricant has very promising future to substitute petroleum based lubricant. Due to sustainability issue, lubricants from natural resources is sought after as complement or even substitute for non renewable lubricants. Jatropha curcas Lin oil (JCO) is one of such natural oil. When tested as lubricant, JCO demonstrates good performance and decomposition properties. The research on JCO usually study the performance the oil by characterizing of friction reduced parameters and rarely to analyze deeper in terms of the role of molecular interaction between components of vegetable oil and metal surfaces. To analyses the moleculer interaction, a commercially available software for molecular interaction simulation is employed. In order to simulate the interactions, the procedure of simulation are firstly construct molecular model of JCO components. The model then is employed as basis for the software to calculate interactive forces of each atom or molecule with the neighboring one thru their positions. From the simulation results, it was concluded that value of dipole moment, polarisability, and bond energy of Jatropha oil compound decreased when the concentration of eugenol is increasing. The conclusion is hold true up to 20% of eugenol additon.

1. Introduction

Friction is often considered as parasitic force which tends to oppose motion or prevent movement. In the machine process, friction occurs due to microscopic contact between the rubbing surfaces (mainly between cutting tool and chips) [1] [2]. This friction may cause an increase in the temperature of the tool and workpiece and cause detrimental effect to the process when not handled wisely. Some machining processes may be conducted in dry machining processes or without coolant, resulting in high temperature in the cutting zone. Even though it works for certain processes, this practice will give very low machining performance in terms of low surface quality and high wear to the tool.

Lubrication in the machining process plays a very important role in improving the performance of the process. Lubricating oil can increase productivity and quality of machining process by providing a lubricating

layer on the cutting zone to reduce friction on the surface. Proper lubrication for boundary regime of lubrication usually takes place when lubricant forms lubricating film on the metal surface. The formed film layer becomes the media for lubricant to reduce friction by preventing direct contact between metal surfaces. The formation of the film is controlled by adsorption process, viscosity, and bond energy.

Most metalworking fluids (MWF) which are used in the machining process are petroleum-based ones. Approximately 85% of the lubricating fluids used worldwide are petroleum-based lubricant [3]. Due to its function, the consumption of MWF is ever increasing in the machining process. It was reported that the European Union itself consumes about 320,000 tons per year, of which at least two thirds need to be recycled [1]. The use of petroleum-based lubricant is very high risk since it may initiate many negative effects on the environment due to its non-renewable issue. It contaminates the surface, groundwater, and the soil [4] [5].

To address this negative effect, various MWF alternatives are being explored by scientists [6] [7]. As a result, alternative MWF may use vegetable oil, especially non-edible ones such as Jatropha curcas Oil [8] [9] [10]. This kind of oil is an excellent alternative for petroleum-based lubricant for MWF because it is eco-friendly, renewable, non-toxic, and biodegradable. However, vegetable oil as lubricants is not as good as lubricants mineral oil based because of it detrimental characteristic [11] [12]. Arguably, the viscosity of vegetable oil is usually lower than petroleum oil [13] [14].

Ones of indicators of good lubricity may be determined by contact angle and its ability to lubricate by wear test [15] [16] [17]. While contact angle is determined by measuring the angle of contact in surface [18] [19], the wear test is conducted by testing the lubrication system using wear tester such as pin-on disk apparatus [20]. Contact angles are very often used to measure or indicate interactions between the lubricant and the surface in which higher contact angle indicate higher viscosity and higher resistance to move [21] [22]. Another approach can be conducted by using simulations methods by employing chemical program applications [23] such as Hyperchem to provide estimation about the interaction between the individual components of lubricating oil, additives, as well as mixture of lubricating oils and additives to affinity into certain surface (such as metal) [24]. This method is still limited in lubrication area therefore study of the effect of the addition of the bio-additive of eugenol [25] to JCO is conducted. It has the objective to analyze intermolecular interactions of mixture of JCO and eugenol information of a film on the surface of the material.

2. Materials and Methods

2.1 The Role of Molecular Interactions in Adsorption of Fatty Acid in Metal Surface

For the machining process, the use of lubricant to improve the frictional conditions hence to avoid excessive heat on the contact point between tool and chips and specimens are recommended. Lubrication regime in machining process depends on the conditions of the process which may falls into one of the lubrication regimes, i.e. boundary, mixed, elasto-hydrodynamic, and hydrodynamic. When, for example, boundary lubrication regime occurs then asperities of two lubricated surface in motion may come into contact in which abrasion or even adhesion occurs.

To reduce boundary lubrication then the correct lubricant viscosity needs to be provided. A lubricant with too high viscosity may increase lubricant's molecular friction while too low one is not so good in separating metal surfaces. Issue in molecular friction make lubricant with too high viscosity has tendency to slide past each other and increase operational temperatures and energy loss. Another way to deal with boundary lubrication is forming sacrificial film between the asperities. Instead of metal surface, the film which able to withstand high pressure and high temperature act as medium so that the surfaces slide over each other.

Since the forming of film is not always constant, then thin film formation (TFL) may occur which only partially covers some asperities. For this kind of film, the properties of lubricants in regards of their molecular structure become important [26]. The relationship between wear and molecular structures of lubricant can be described by simulation on the adsorption of metal surface (adsorbent) and fatty acid (adsorbate) [27] [28] [29] [30]. Therefore, studying molecular interactions is very important to understand the adsorption mechanism between adsorbate and adsorbent as in adsorption of fatty acid in metal surface.

Adsorption may occur in two categories, which are psysisorption and chemisorption. While physisorption mainly involves weak van der Waals interactions, chemisorption involves attraction to the surface by formation of chemical bonds. Molecular interactions between two or more molecules or either two atoms are likely occurred at the site which has highest and opposite charges. Also, it occurred at two atoms which have the highest density in their highest occupied molecular orbital, HOMO/LUMO interaction [31]. Also, other parameters such as dipole moment, bond energy and heat of bond formation are used as the basis for determining the level of adsorption [32]. In general, the molecular orbital energy level expressed in Highest Occupied Molecular Orbital (HOMO) and Lowest Un-occupied Molecular Orbital (LUMO) will express the adsorption level of each fatty acid that forms JCO. To calculate HOMO+ and LUMO-, the semi-empirical MINDO/3 method may be used [33], which is available in commercial computer programs such as Hyperchem 8.0.

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Dipole moments, bonding energy, charge density, and electrostatic potential are some of the parameters which describe Van der Waals forces which contribute to the adsorption energy. The affinity of a fatty acid for a certain adsorbent (metal surface) depends on certain characteristics as such polarity, shape, size, and partial pressure or concentration in the fluid, and system temperature [31]. The very simple approach to calculate the parameters using only molecular mechanics and structure using straight molecular conformer shows very interesting results. Also, the wear test to support the simulation result to contact angle and wear also was presented [34].

2.2 Molecular Dynamic Model and Simulation Process

The molecular model of JCO as lubricating oil was constructed by using Hyperchem 8.0. Since the oil has a certain composition of fatty acids then the constituent for the oils were given in Table 1. The simulation of molecular interactions is conducted by using a commercially available simulation software. The computer has the processor of an Intel Core i7 2.7 GHz and 8 GB 2133 MHz DDR4 RAM. The software takes a straightforward approach for the molecular dynamic simulation process. When the positions of all the atoms which compose a system of molecules or groups of molecules which interact each other are known, then forces experienced by an atom in the molecules can be calculated because of its interactions with neighboring atoms.

Table 1 *Composition of Jatropa curcas Lin. oil*

Fatty acids constituent of Jatropa curcas Lin. Oil (JCO) [1]	
Fatty acid	Percentage (%)
Ricinoleic acid	86
Dihydroxy stearic acid	1-2
Stearic acid	0.5-2.0
Oleic acid	8.5
Linoleic acid	3.5

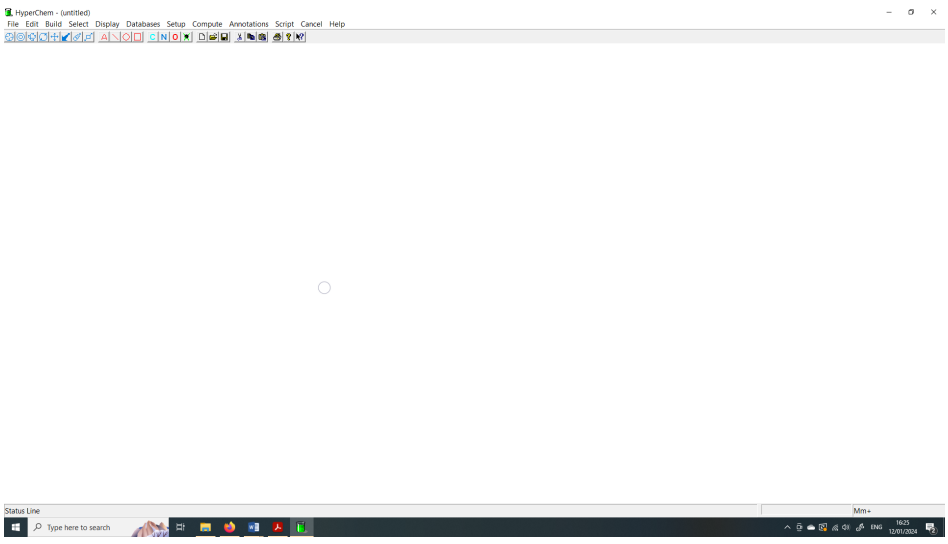


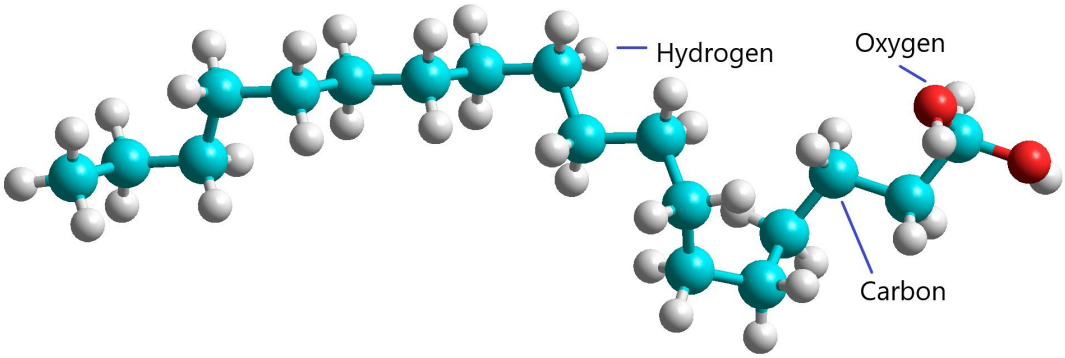
Fig. 1 *Screenshot of Hyperchem 8.0*

For this simulation, each interacting oils are represented by its constituent components, i.e. fatty acid. Jatropha curcas oil has its constituent fatty acids which are ricinoleic acid up to 86%, then stearic acid (18:2n-6) up to 1-2%, and Stearic acid up to 0.5-2.0%. Another fatty acid is oleic acid of 8.5% and linoleic acid up to 3.5%. Since the fatty acids in the software can only represent a molecular structure thru an image then it will be converted by the Hyperchem 8.0 software into a number. Therefore, computation is started by drawing of the rpresentation of the chemical structure which constitue fatty acid of lubricant. The chemical structure will represents bonding of the atoms in a three-dimensional plane in it most optimal structural form. To have this optimal value, then iterative computation of state of molecular mechanics is conducted until it has a state of small changes in bond angles and stretching while do not make its energy change too sharp. This condition is defined by Root Mean Square (RMS) parameter thru steepest gradient methods in searching for convergence. To

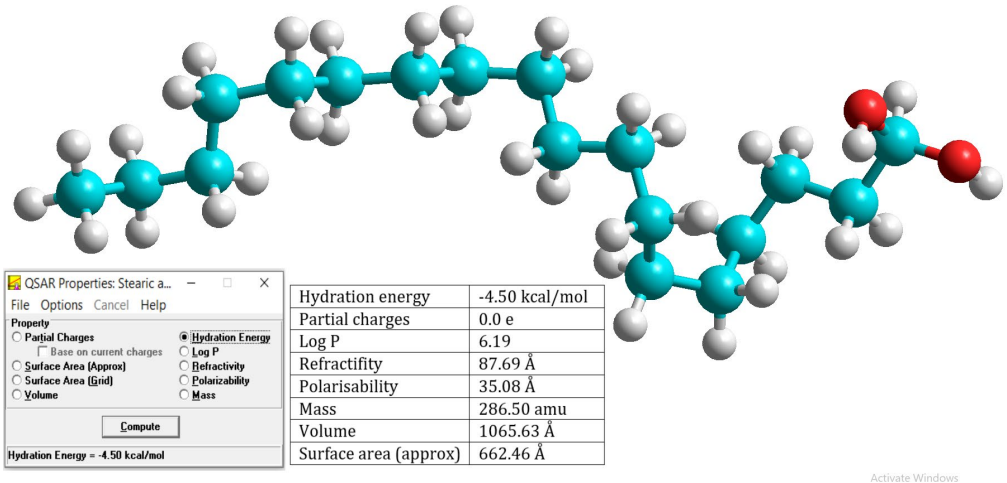
represent the molecules, the software use numeric parameter in regards of the number of atoms, molecular surfaces and other parameters. The model used for the purpose is the quantitative-structure property relations (QSPR) modeling method.

Since to the research also find other parameters such as dipole moment, polarizability, etc., then semi-empirical methods is employed. The method used here are the DFT method or PM3 method. The previously stated parameters of the molecules can be calculated by knowing its charge density thru rooting of the wave function by density functional theory (DFT). The results provide an excellent way to present those parameters thru spectral data and molecular geometry. The drawback of this method, however, lie on the very time consuming simulation when applied to the large and complex moleculer structure. For cases like this, another preferably methods such as parametrized method 3 (PM3) will be much suitable. PM3 will execute the simulation faster in terms of calculations in expense of the accuracy which is lower than DFT. This methods is more suitable for this research since the simulations are running on personal computer with its hardware limitations.

After drawing of fatty acid molecule is drawn, then the simulation will give a results on the parameters in search such as molecular energy, dipole moment, inducible dipole moment, and others. Figure 2, provide examples of the computational steps after 3D images of molecular structures of fatty acid is provided. After this step, the structures is then optimized (relaxed) with the QSAR molecular mechanics method to obtain the energy required for optimization (relaxed) to the state of moleculer structure and also other parameters. To determine the adsorption of each fatty acid component, parameters such as dipole moment, bond energy and total polarizabilty are used as the basis for determining the level of adsorption [32] [26].



(a)



Hydration energy	-4.50 kcal/mol
Partial charges	0.0 e
Log P	6.19
Refractifity	87.69 Å
Polarisability	35.08 Å
Mass	286.50 amu
Volume	1065.63 Å
Surface area (approx)	662.46 Å

(b)

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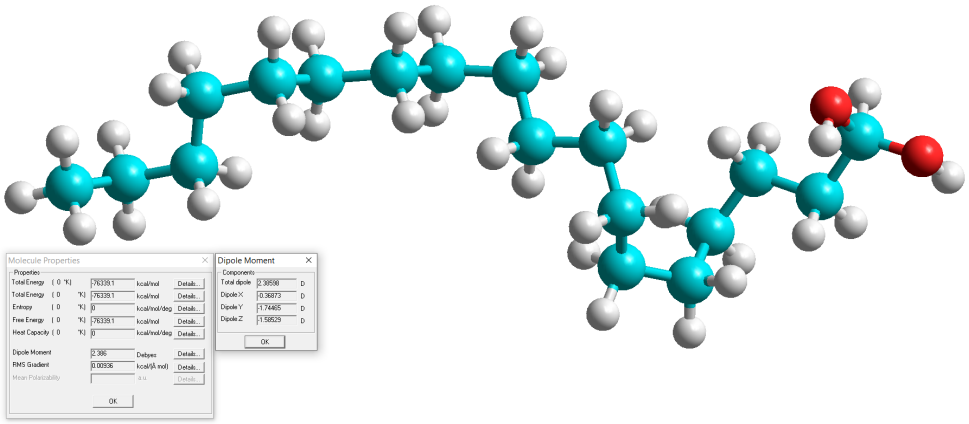

(c)

Fig. 2 *(a) Representation of 3D – molecular structure; (b) Optimized (relaxed) structure by QSAR methods; (c) Energy required to optmize (relaxed) using QSAR*

3. Results and Discussion

3.1 Simulation on Molecular Dynamic

The results of simulation are given in Figure 1, Figure 2, Figure 3, Figure 4 and Figure 5 which shows the electric potential and total charge density of the two mixtures, i.e. JCO and eugenol. Other parameter, the polarizability of the mixture of Jatropha oil and eugenol, as simulated was shown in table 2. Intermolecular forces of the mixture of JCO and eugenol with copper surfaces was simulated and the results is shown in Table 2. Figure 6 depicts the value of the dipole moment for varied concentration of the mixture of JCO and eugenol. The x-axis is the concentration of eugenol added to the JCO. The y-axis is the value of the dipole moment in debyes. At a concentration of 3% the value of the dipole moment is of 18.027 debyes, then concentration of 5% the value of the dipole moment is of 17.133 debyes. Also, at a concentration of 10% the value of the dipole moment is of 8.821 debyes, and finally at a concentration of 15% the value of the dipole moment is of 7.647 debyes. The dipole at a concentration of 20% is 5.465 debyes, and at a concentration of 25% the value of the dipole moment is 2.5 debyes. The trend shows when the eugenol fraction of the mixture higher then the dipole moment become lower.

According to the basic theory, the dipole moment is influenced by the electronegativity of a molecule. Eugenol molecule has the chemical formula C10H12O2. Meanwhile, Jatropha's oil risinoleic acid has the chemical formula C18H34O3. Since O atom has a higher electronegativity than the H atom and C atom, then the more O atoms with a high electronegativity value will make the dipole moment become higher. When the eugenol is added to nixture then the amount of total O become lower and will make dipole moment become lower. Graphically, the relationship between the eugenol fraction and the dipole moment is given in Figure 6.

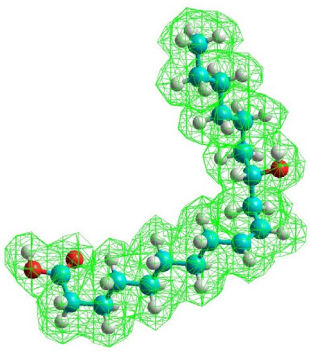

Fig. 3 *Molecular structure and electrostatic potential of ricinoleic acid*

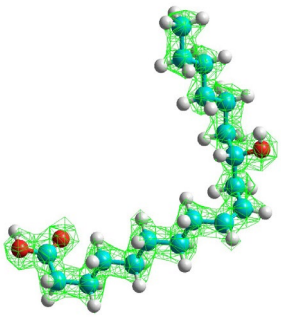

Fig. 4 *Molecular structure and total charge density of ricinoleic acid*

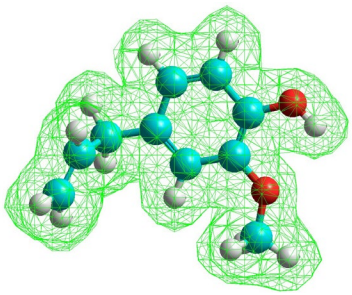

Fig. 5 *Molecular structure and electrostatic potential of eugenol*

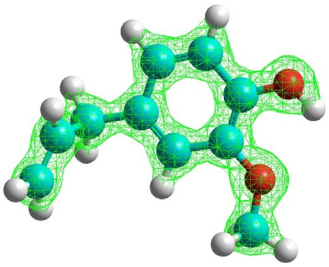

Fig. 6 *Molecular structure and total charge density of eugenol*

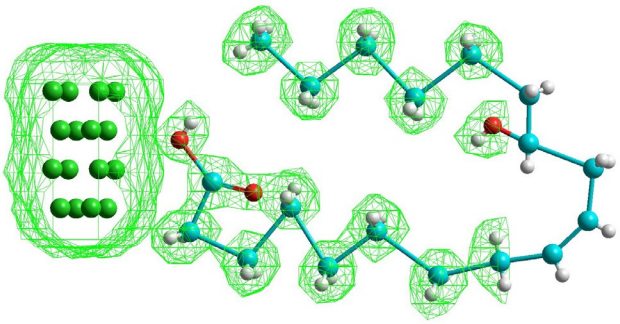

Fig. 7 *Electrostatic potential between ricinoleic acid and copper FCC crystals*

Table 2 *Polarizability of the mixture of Jatropha oil and eugenol*

Percentage	Dipole Moment (Debye)	Total Polarizability (Å^3)	Bonding Energy (kJ/mol)
JCO+3%E	26.108	584.21	-359104.128
JCO+5%E	15.123	303.78	-206976.029
JCO+10%E	8.622	155.78	-98987.629
JCO+15%E	7.451	123.35	-76917.328
JCO+20%E	5.354	87.78	-54861.255
JCO+25%E	2.442	53.21	-32626.874

Table 3 *Intermolecular force of the mixture of Jatropha oil and eugenol*

Mixture of JCO & E + Copper (FCC)	Bonding Energy (kJ/mol)
JCO+3%E + Copper	-141585.160
JCO+5%E + Copper	-132655.561
JCO+10%E + Copper	-110331.563
JCO+15%E + Copper	-87998.867
JCO+20%E + Copper	-64672.706
JCO+25%E + Copper	-42998.897

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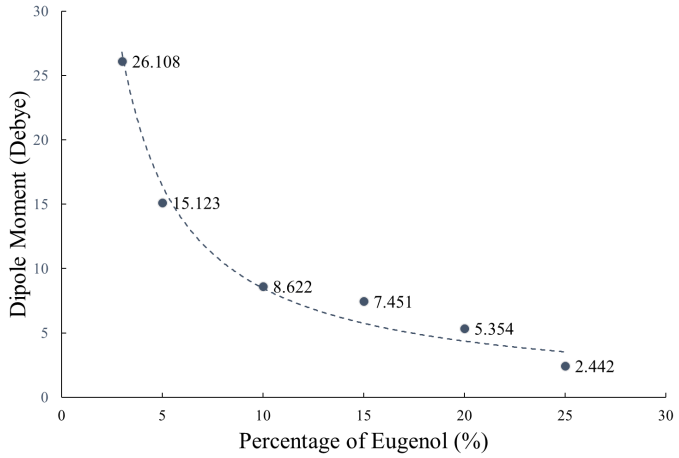

Fig. 8 *Eugenol fraction to dipole moment*

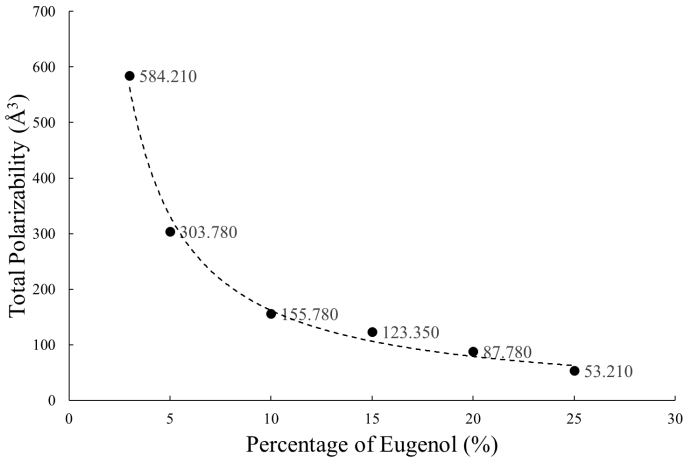

Fig. 9 *Eugenol fraction on polarisability*

Figure 7 shows the polarisability for the addition of eugenol into the JCO to make a mixture of lubricant. The x-axis shows the variation of the concentration of eugenol while the y-axis shows the value of polarisability of the mixture , eugenol and Jatropha oil, in units of Å3. The dotted blue line shows the trend of the data from the value of polarisability to the eugenol concentration. At a concentration of 3% eugenol the polarisability value was 581.18 Å3, concentration of 5% eugenol gives a polarisability value of 333.90 Å3, concentration of 10% eugenol obtained a polarisability value of 160.95 Å3, concentration of 15% eugenol had a polarisability value of 125.43 Å3, then concentration of 20% eugenol resulted in a polarisability of 89.90 Å3, and 25% eugenol obtained a polarisability value of 54.38 Å3.

Polarisability is the ability of a molecule to form or induce dipole moment. Polarisability is influenced by the value of the relative atomic mass (Mr) and the shape of the structure of a molecule. The higher the Mr value of a molecule, the higher the polarisability value will be. The longer the shape of the structure of a molecule, the higher the polarisability value will be. Figure 8 shows the bonding energy value to the addition of Eugenol concentration into Jatropha Oil. The x-axis is the concentration of eugenol added to Jatropha Oil, while the y-axis represents the bonding energy between eugenol and Jatropha Oil molecules in kJoule/mol units. The dotted blue line shows the tendency of the bond energy values (kJ/mol) to the addition of eugenol concentration.

At a concentration of 3% eugenol, the bond energy value is -361094.137 kJ/mol, at 5% eugenol, the bond energy value of -207079.038 kJ/mol, at 10% eugenol, the bond energy value of -99382.523 kJ/mol. 15% eugenol the bond energy value obtained is -77015.219 kJ/mol, at 20% eugenol bond energy value is -54861.255 kJ/mol, and at 25% eugenol the bond energy value is -32626,874 kJ/mol. Bond energy can also be defined as the amount of energy required by a molecule to form/separate a certain chemical bond. Bond energy is negative in value accordance to the law of conservation of energy, because when a bond is formed the energy from its formation is stored in the bonds between atoms.

Figure 9 shows the value of bond energy for the addition of eugenol into Jatropha Oil on 1x2x2 unit of copper crystals. The x-axis shows the variation in concentration of eugenol added to Jatropha Oil while the y-axis shows the value of the bonding energy between the molecules of eugenol and Jatropha Oil on Copper crystals in units of kJoule/mol. The blue dotted line shows the tendency of the data from the bond energy values in kJ/mol of the addition of eugenol concentration to Jatropha oil.

At a concentration of 3% eugenol, the bond energy value is -141585.16 kJ/mol, for a concentration of 5% eugenol, the bond energy value was -132655.561 kJ/mol. For 15% eugenol bond energy value obtained is -88007.565 kJ/mol, for 20% eugenol the bond energy value is -65591.706 kJ/mol, and at 25% eugenol obtained bond energy value is -43195.298 kJ/mol.

The bond energy on the surface of a material is influenced by molecular interaction forces such as the Van der Waals force and hydrogen bonds, as well as the surface free energy of a material. The bond energy that control of the binding of molecules to the surface of the material can be utilize a marker of the ability of a compound (absorbate) to stick to the surface of the material (absorbent). The value of the bond energy also indicates molecular interaction force that occurs therefore higher bond energy refers to gather with itself. The value of the bond energy is influenced by the dipole moment and the polarity of the compound molecule, where the value is directly proportional.

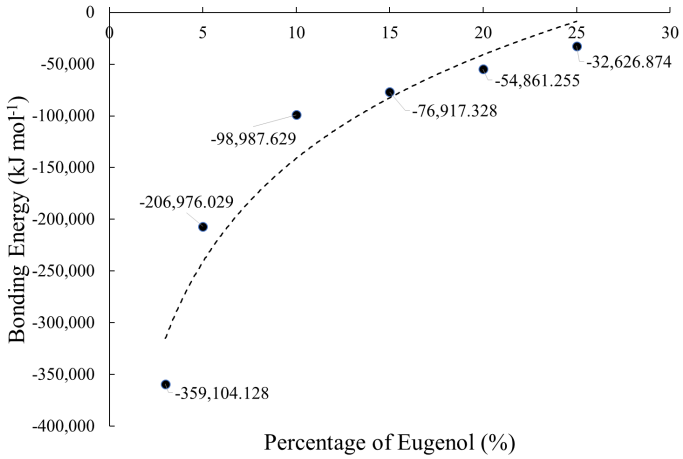

Fig. 10 *Eugenol fraction to bond energy*

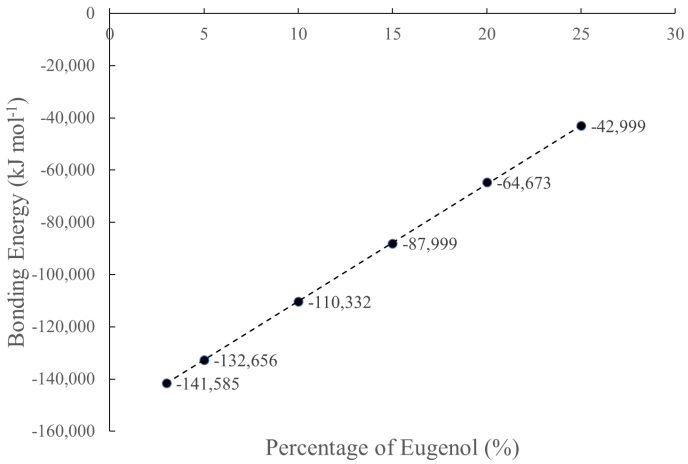

Fig. 11 *Eugenol fraction on bond energy with copper crystals*

3.2 Contact Angle Measurement

The contact angle measurement on glass for mixture of eugenol and JCO is given in Table 2. The measurement shows that the larger of eugenol composition makes the contact angle of the mixtures become lowest. It was known that the viscosity of JCO is higher than eugenol, therefore the contact angle of mixture will follow the viscosity of mixture. The lower contact angle will give better wetting properties.

Table 4 *Contact angle of mixtures of eugenol and Jatropa curcas Lin. oil*

Mixture of Eugenol & JCO	Contact angle (degree)
3% Eugenol + 97 % JCO	23.5
5% Eugenol + 95 % JCO	19
10% Eugenol + 90 % JCO	15

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20% Eugenol + 80 % JCO	13
30% Eugenol + 70 % JCO	13

4. Conclusion

From the results and discussion, it can be concluded that the value of the parameters of molecular interaction affects the physical properties of the lubricant. The bond energy is directly proportional to tendency of the molecules to stick on the surface of material. The surface wettability of the material (absorbent) is influenced by the surface free energy and the intermolecular interaction forces on the absorbate molecules. The higher energy difference between a molecule and the absorbate then better the adsorption to the absorbent surface. One of the possibility of this condition is achieved when the molecular energy of the lubricant decreases and the free energy of the metal surface remains or increases. It is also found that the value of dipole moment, polarisability, and bond energy of mixture decreased with the increase in the concentration of eugenol. This iphenomena is related to non-polar mixture of Jatropha oil and eugenol, so that the electronegativity and polarity levels are low, resulting in a lower bond energy. From the simulated value of the dipole moment, polarisability, and bond energy, it can be concluded that the addition of the eugenol is expected to increase the lubricating properties of Jatropha oil due to the increase in wetting of the metal surface by lubricant. This is indicated by the decrease in the bond energy in lubricant molecules compounds so that the affinity against copper crystals increases.

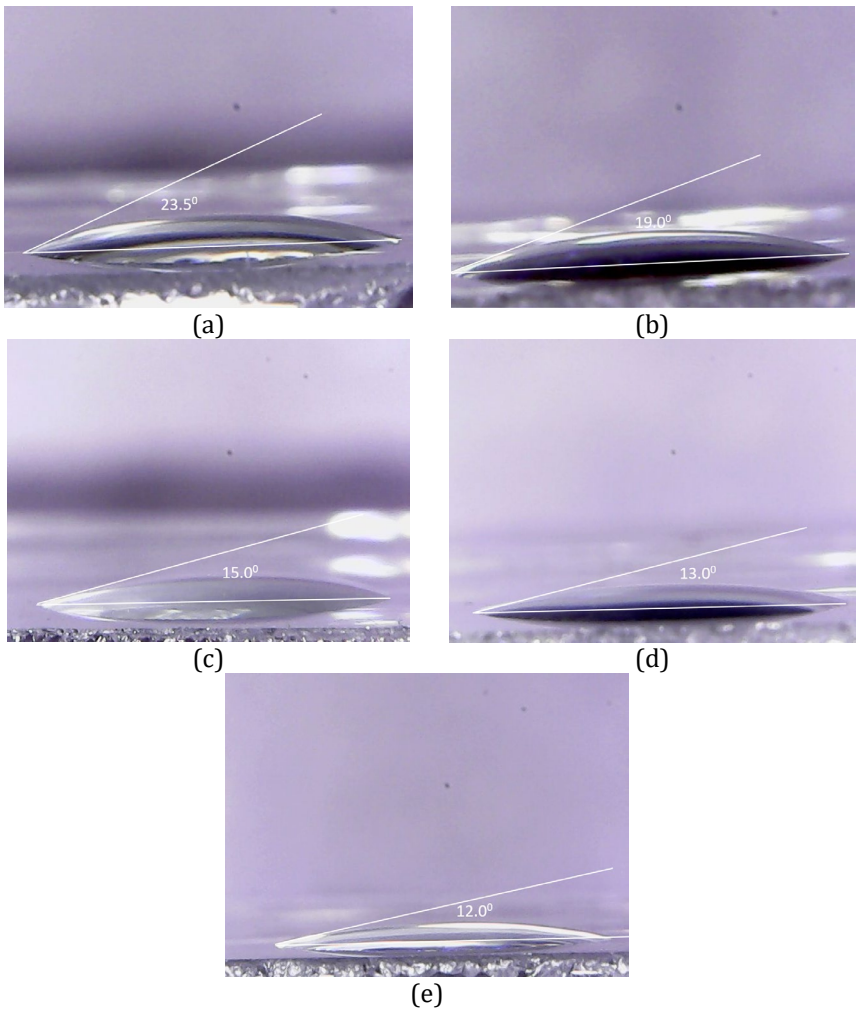

Fig. 12 *Contact angle measurement of mixture of eugenol and Jatropa curcas Lin. Oil, (a) 3% eugenol and 97% JCO; (b) 5% eugenol and 95% JCO; (c) 10% eugenol and 90% JCO; (d) 20% eugenol and 80% JCO; (e) 30% eugenol and 80% JCO*

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Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

Author Contribution

Study conception and design: *MSM. IGNW, DBD, ON;* ***data collection:*** *CHD, MSM Author Y;* ***analysis and interpretation of results:*** *MSM, CHD, P;* ***draft manuscript preparation:*** *MSM, IGNW, ZA. All authors reviewed the results and approved the final version of the manuscript.*

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