Simulation of the Influence of Eugenol ($C_{10}H_{12}O_2$) on *Jatropha curcas* Linn. Oil to Improve Physical Properties of Base Oil

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Abstract. Lubrication in machining process plays a very important role in machining because it increases the productivity and quality of the machining process. Today, most Metalworking Fluids (MWF) are petroleum based ones. Due to its advantages, the consumption of MWF is increasing therefore creating many negative effects on the environment. These effects are related to surface and groundwater, and soil contamination. To address this challenge, various MWF alternatives are being explored by scientists. Vegetable oil is a very attractive alternative to petroleum-based lubricants, because vegetable oils are environmentally friendly, renewable, non-toxic, and easily biodegradable. In complement to the experimental method, simulations using chemical application programs such as Hyperchem 8.0 can also be carried out to provide an estimate of how the interaction between components of lubricating oil, lubricating oil and additives, as well as lubricating oil and additives to their attraction properties to certain surfaces (such as metals). In this study, the effect of the addition of eugenol as a bio-additive on the interaction between molecules of jatropha oil lubricant on the surface of the material will be analysed. The results obtained are simulations using Hyperchem 8.0 can be used to predict the physical properties of the lubricating oil.

Keywords: Energy, lubricant, molecular interaction, vegetable oil.

1 Introduction

Friction is a force that opposes motion or prevents movement. On machining process, friction occurs due to microscopic contact points that occur between the rubbing surfaces (chisel and chips) [1]. Friction between chisel and chips can cause an increase in the

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temperature of the tool and workpiece surface [2, 3]. Condition dry machining processes or without coolant, resulting in high temperature in the cutting zone, resulting in high performance very low machining resulting in decreased surface quality workpiece and tool used [4, 5].

Lubrication in machinery plays a very important role in improving performance machining. Lubricating fluids can increase productivity and process quality machining [6]. Lubricating fluid is a liquid used during the process machining capable of providing a lubricating layer on the cutting zone in order to reduce friction on the surface [7, 8].

Lubrication can occur properly if the lubricating fluid can form film on the metal surface [9]. The film layer that is formed becomes the media a lubricant that reduces friction by preventing direct contact between metal surface [10]. The formation of the film layer by the lubricating fluid is affected by adsorption process, viscosity and bond energy [11].

Most Metalworking Fluids (MWF) are fluids petroleum based [12]. Approximately 85 % of the lubricating fluids used worldwide, petroleum-based [12]. Due to its function, the consumption of MWF increase in the machinery industry. It was reported that the European Union itself consumes about 320 000 t yr^{-1}, of which at least two thirds is necessary discarded [13]. The use of petroleum is very large, creates many negative effects on the environment. The main negative effects are related with surface and groundwater contamination, and soil contamination [14].

To address this challenge, various MWF alternatives are being explored by scientists and tribologists. As a result, the MWF alternative can use vegetable oil [15, 16]. Vegetable oil is an excellent alternative attractive for petroleum-based coolants, that's because MWF is oil-based eco-friendly, renewable, non-toxic and biodegradable. As a result, nowadays, vegetable oil is a potential alternative to use in the cooling/MWF industry [17, 18].

However, until now vegetable oil lubricants are not as good as lubricants mineral oil based. This is partly due to the value of very low viscosity. Previous research shown that the viscosity value of vegetable oil is lower than with mineral oil lubricants [19]. For this reason, more research is needed further in order to produce lubricating compounds based on vegetable oils that well, in order to compensate for the abundance of vegetable oil resources and reduce the negative effects of excessive use of mineral oil.

To determine the adhesive properties of the lubricant, the method of measuring the angle, contact angle measurement is very often used to measure interactions between the lubricant and the surface. In addition, simulations using the program chemical applications such as Hyperchem can also be performed to provide estimates about how the interaction between the components of fuel [20] lubricating oil, lubricating oil and additives, as well as lubricating oils and additives to their surface affinity to certain surface (such as metal) [21]. Because there is still little research in the Department of Mechanical Engineering related to this simulation it is necessary to start research with using simulation in the field of lubrication.

In this study, the effect of the addition of the bioadditive eugenol will be analyzed to the intermolecular interactions of castor oil lubricants that affect the formation of a film on the surface of the material.

2 Materials and method

This research uses Hyperchem 8.0 software which is available for free on the internet. HyperChem 8.0 simulation software is a molecular modeling and simulation software that makes it possible to perform complex chemical calculations using a computer. The steps taken in this simulation are to design fatty acids and other components used in this study using HyperChem 8.0 software. Furthermore, this study simulates the molecular reaction of

ricinoleic acid, linoleic acid, palmitic acid with eugenol, and copper FCC crystals to obtain the properties of each molecule with HyperChem 8.0.

After the molecular structure is drawn, the next step is to optimize the molecular geometry in order to obtain the results of the minimum atomic energy and force values in the system and improve the molecular distance so that it is homogeneous with one another. After the geometry optimization process is complete, then proceed to the following steps: molecular dynamics. This step is used to set the simulation temperature according to the controlled variable.

The next step was to find the following: dipole moment, polarizability, bond dissociation energy of oil components, and between mixture of *Jatropha curcas* Linn. oil and eugenol with copper crystals.

3 Result and discussion

Simulation results are shown 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.

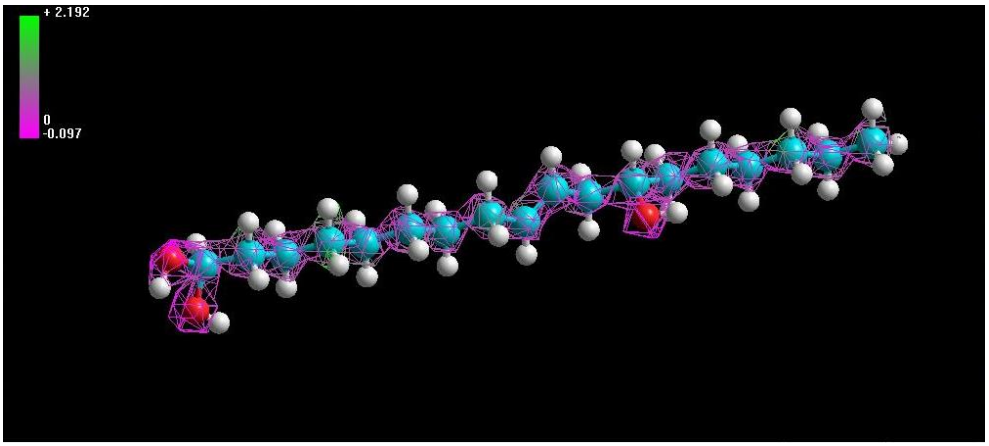

Fig. 1. Molecular structure and electrostatic potential of ricinoleic acid.

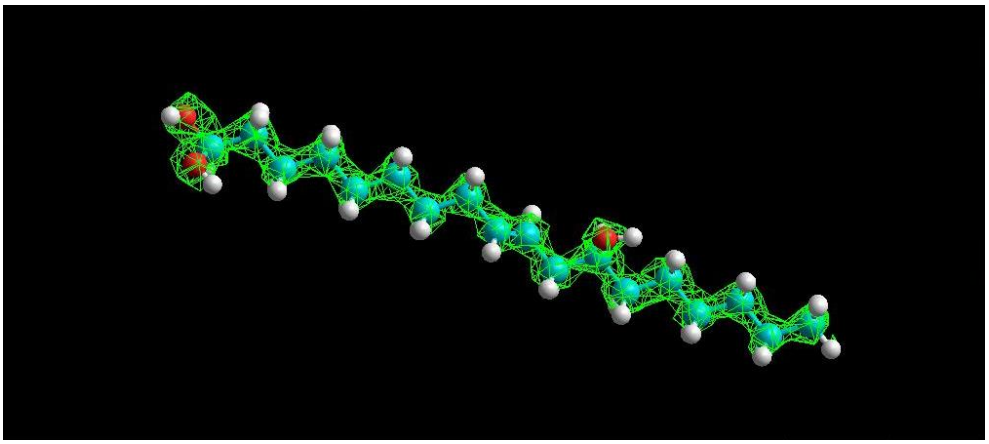

Fig. 2. Molecular structure and total charge density of ricinoleic acid.

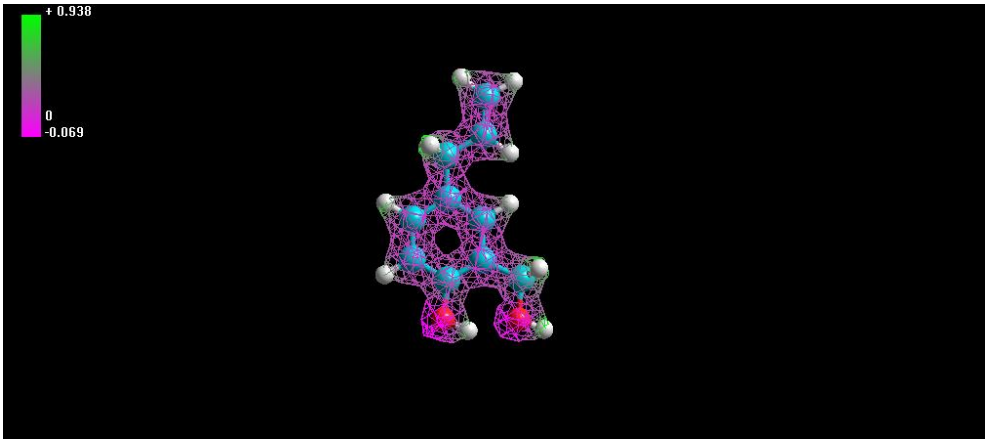

Fig. 3. Molecular structure and electrostatic potential of eugenol.

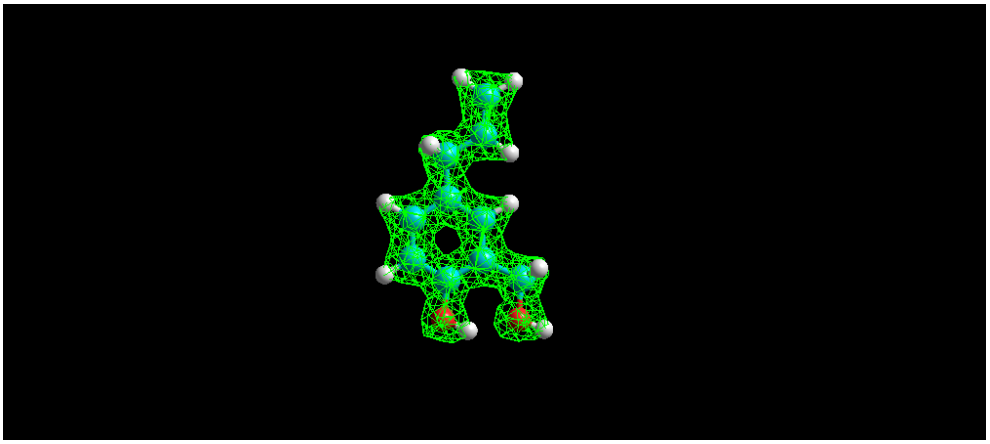

Fig. 4. Molecular structure and total charge density of eugenol.

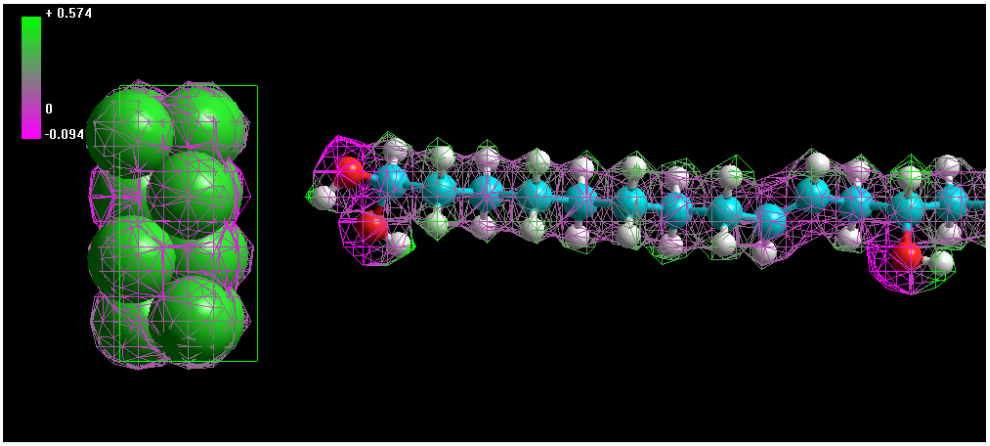

Fig. 5. Electrostatic potential between ricinoleic acid and copper FCC crystals.

Next, the polarizability of the mixture of jatropha oil and eugenol as simulated was shown in Table 1.

Table 1. Polarizability of the mixture of jatropha oil and eugenol.

Percentage	Dipole moment (Debye)	Total polarisability (Å^3)	Bonding energy (kJ mol^{-1})
JCO + 3 % E	28.207	581.18	-361 094.137
JCO + 5 % E	17.133	333.90	-207 079.038
JCO + 10 % E	8.821	160.95	-99 382.523
JCO + 15 % E	7.647	125.43	-77 015.219
JCO + 20 % E	5.465	89.90	-54 861.255
JCO + 25 % E	2.5	54.38	-32 626.874

Also intermolecular forces of castor oil and eugenol with copper surfaces was simulated and the results is shown in Table 2.

Table 2. Intermolecular force of the mixture of jatropha oil and eugenol.

Mixture of JCO & E + Copper (FCC)	Bonding Energy (kJ mol^{-1})
JCO + 3 % E + Copper	-141 585.160
JCO + 5 % E + Copper	-132 655.561
JCO + 10 % E + Copper	-110 331.563
JCO + 15 % E + Copper	-88 007.565
JCO + 20 % E + Copper	-65 591.706
JCO + 25 % E + Copper	-43 195.298

Graphically, the relationship between the eugenol fraction and the dipole moment is given in Figure 6.

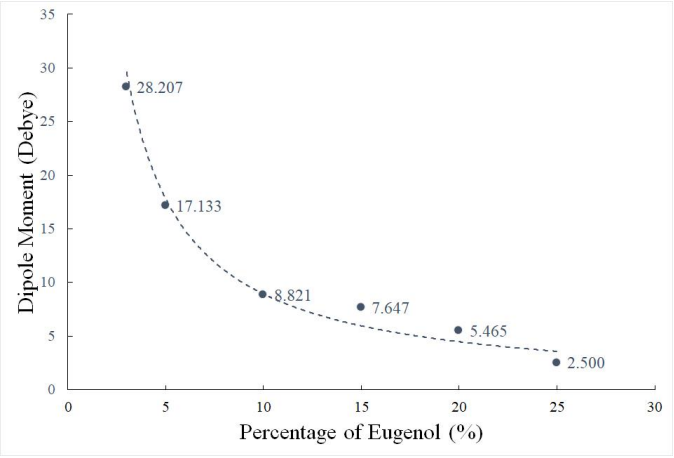

Fig. 6. Eugenol fraction to dipole moment.

Figure 6 shows a graph of the value of the dipole moment for the addition of eugenol concentration into the jatropha oil. The X axis shows the variation in the concentration of eugenol added to the castor oil liquid. The Y axis shows the value of the dipole moment in Debyes units. The yellow dotted line indicates the tendency of the dipole moment value to the eugenol concentration.

At a concentration of 3 % the value of the dipole moment is 18.027 Debyes, at a concentration of 5 % the value of the dipole moment is 17.133 Debyes, at a concentration of 10 % the value of the dipole moment is 8.821 Debyes, then at a concentration of 15 % the value of the dipole moment that occurs is 7.647 Debyes, the value of the moment is

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.

According to the basic theory, the dipole moment is a polarity that is influenced by the electronegativity of a molecule. Eugenol molecule has the chemical formula $C_{10}H_{12}O_2$. Meanwhile, jatropha's oil risinoleic acid has the chemical formula $C_{18}H_{34}O_3$, where the O atom has a higher electronegativity than the H atom and C atom. So, the more O atoms with a high electronegativity value, the higher the dipole moment involved will also be where in ricinoleic acid there are more O atoms.

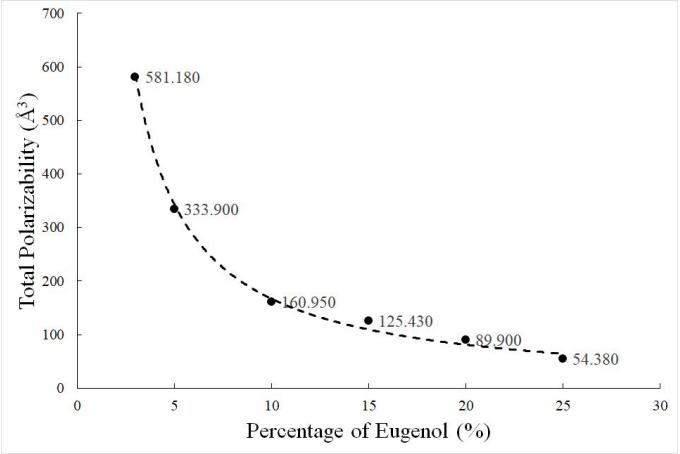

Fig. 7. Eugenol fraction on polarisability.

Figure 7 shows a graph of the polarisability value for the addition of eugenol concentration into the jatropha oil. The X axis shows the variation of the concentration of eugenol addition into jatropha oil. While the Y axis shows the polarisability value that works on a mixture of eugenol and jatropha in units of three. The dotted blue line shows the trend of the data from the polarisability value to the eugenol concentration.

At a concentration of 3 % the polarisability value was 581.18 Å^3, a concentration of 5 % with a polarisability value of 333.90 Å^3, a concentration of 10 % obtained a polarisability value of 160.95 Å^3, a concentration of 15 % had a polarisability value of 125.43 Å^3, concentration 20 % resulted in a polarisability of 89.90 Å^3, and 25 % obtained a polarisability value of 54.38 Å^3.

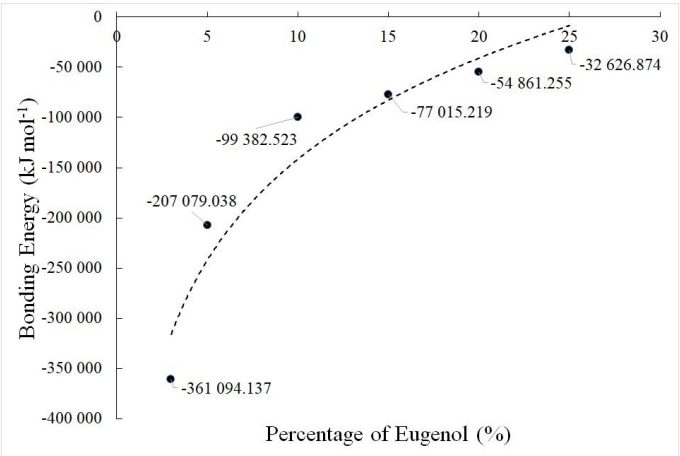

Fig. 8. Eugenol fraction to bond energy.

According to the basic theory, polarisability is the ability of a molecule to form or induce a dipole to form a temporary dipole. Polarisability is also 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 and longer the shape of the structure of a molecule, the higher the polarisability value will be.

Figure 8 shows a graph of the bonding energy value to the addition of eugenol concentration into jatropha oil. The X axis shows the variation in the concentration of eugenol added to jatropha oil. While the Y axis shows the value of the bonding energy that occurs between eugenol and jatropha oil molecules in kJ mol^{-1} units. The dotted orange line shows the tendency of the data from the bond energy values to the addition of eugenol concentration.

At a concentration of 3 %, the bond energy value was -361 094.137 kJ mol^{-1}, at 5 % concentration, the bond energy value was -207 079.038 kJ mol^{-1}, at 10 % concentration, the bond energy value was -99 382.523 kJ mol^{-1}. 15 % bond energy value obtained is -77 015.219 kJ mol^{-1}, 20 % concentration obtained bond energy value is -54 861.255 kJ mol^{-1}, 25 % concentration obtained bond energy value is -32 626.874 kJ mol^{-1}.

According to the basic theory, bond energy can also be defined as the amount of energy required by a molecule to separate a certain chemical bond. Bond energy is negative in accordance with the law of conservation of energy, because when a bond is formed the energy from its formation is stored in the bonds between atoms.

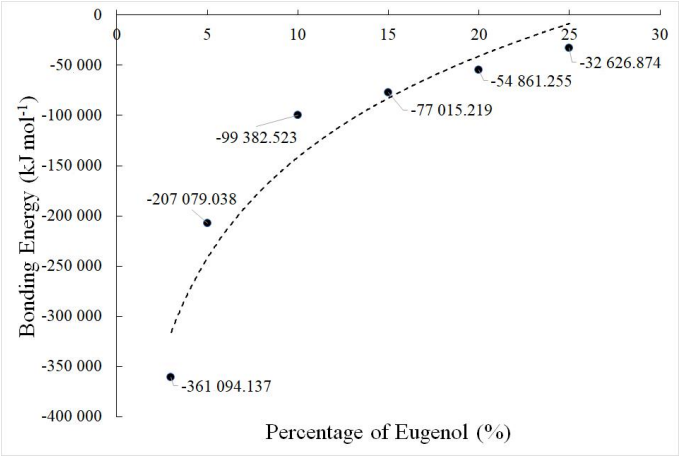

Fig. 9. Eugenol fraction on bond energy with copper crystals.

Figure 9 shows a graph of the bond energy value of the addition of eugenol concentration into castor oil on 1 × 2 × 2 unit copper crystals. The X axis shows the variation in the concentration of eugenol added to castor oil. While the Y axis shows the value of the bonding energy that occurs between the molecules of eugenol and castor oil on copper crystals in units of kJ mol^{-1}. The green dotted line shows the tendency of the data from the bond energy values to the addition of eugenol concentration.

At a concentration of 3 %, the bond energy value was -141 585.16 kJ mol^{-1}, for a concentration of 5 %, the bond energy value was -132 655.561 kJ mol^{-1}. For concentration of 10% the bond energy value was -110 331.563 kJ mol^{-1}, 15 % bond energy value obtained is -88 007.565 kJ mol^{-1}, 20 % concentration obtained bond energy value is -65 591.706 kJ mol^{-1}, 25 % concentration obtained bond energy value is -43 195.298 kJ mol^{-1}.

According to the theoretical basis, 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 binds to the surface of the material can be a marker of the ability of a compound (absorbate) to stick to the surface of the material (absorbent). The greater the value of the bond energy, it also indicates that the molecular interaction force that occurs is more and more so that it prefers 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.

4 Conclusion

From the results and discussion, it can be concluded 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 the energy difference, in negative term, between a molecule and the absorbate then better the attachment to the absorbent surface. This is achieved when the molecular energy of the lubricant decreases, *i.e.* more negative, 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 jatropha oil lubricating compound decreased with the increase in the concentration of eugenol. This is because the mixture of jatropha oil and eugenol molecules produces non-polar compounds, so that the electronegativity and polarity levels are low, resulting in a lower bond energy.

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