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STUDY OF THE INTERESTERIFICATION PROCESS OF PALM OIL INTO METHYL ESTERS WITH BIOCATALYSTS OF AROMATIC COMPOUNDS

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Abstract. The interesterification reaction of palm oil and methyl acetate to produce methyl ester and triacetin was conducted with biocatalysts of aromatic compounds, namely eugenol and cajuput oil. Aromatic compounds are the most efficient catalysts in the manufacturing process of biodiesel, leading to improved quality. Therefore, this study aimed to obtain a more effective and efficient biodiesel production process, with fewer procedural steps, in order to reduce production costs. The operating conditions of the study included 250 g of palm oil mass, a molar ratio of palm oil to methyl acetate at 1:6, a reaction temperature of 60°C, 300 rpm stirring speed, the catalyst mass of 0.75% palm oil mass, as well as reaction time of 15, 30, 45, 60, and 75 minutes. The molecular behaviour and parameters were the bond distance between atoms before and after the addition of the biocatalyst, potential energy, kinetic energy, and dipole moment, determined by the simulation using ChemDraw software.

Keywords: interesterification, aromatic compounds, catalyst, kinetic energy, dipole moment.

1. Introduction

The predominant method used for the production of biodiesel is the transesterification process. However, a significant disadvantage of this process is the relatively challenging separation required for the generated glycerol by-product. The presence of glycerol in biodiesel poses a risk of disrupting engine performance. An alternative approach to biodiesel production includes deviating from the traditional alcohol-based reaction route to a non-alcoholic pathway known as interesterification. In the alcohol route, methanol is used to supply alkyl groups, while in the non-alcoholic route, it is replaced by methyl acetate as a methyl group supplier. Examining the reactions that occurred, the byproducts from the non-alcoholic and alcoholic routes were triacetin and glycerol, respectively.[1] Triacetin is an additive in foods such as candy, dairy drinks, chewing, and flavoured drinks.[2] It is used as a solvent in the perfume industry, printing ink, solvent for fragrance, plasticizer for cellulose resins, polymers, and copolymers, as well as additives in car engines, thereby increasing the economic value of biofuels and even glycerol.[3,4] Triacetin is also used as a fuel additive to reduce knocking in car engines and reduce emissions.[4,5] Moreover, incorporating it into biodiesel at a 10% concentration yields a final product that upholds a commendable quality standard.[6]

A study on the interesterification process commonly incorporates a catalyst to accelerate the reaction, except in supercritical conditions with elevated temperature and pressure. In the process using homogeneous catalysts, a neutralization reaction stage is essential, followed by the separation of the reaction products.[7,8] Conversely, heterogeneous catalysts necessitate an activation stage and catalyst separation, thereby extending the process stages and inevitably increasing production costs.[9–11] Aromatic compounds, such as benzene (C_6H_6) contain aromatic groups characterized by delocalized molecular orbitals. The resulting electron delocalization imparts stability and inertness to the compound. In aromatic compounds, it generates a magnetic field that will affect the stability of polar compounds.

The utilization of the magnetic properties of heterogeneous catalysts in biodiesel production has shown satisfactory outcomes. In the study of the transesterification of used cooking oil by adopting the magnetic properties of the $CuFe_2O_4$ catalyst, a 93% yield was achieved at a

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reaction time of 90 minutes.[12] Simultaneous transesterification and esterification using Fe_3O_4/SiO_2 led to a conversion of 93% with a reaction time of 6 hours.[13] The production of biodiesel from the transesterification of Pistacia Chinensis seed oil with a cellulose magnet catalyst yielded 93.1% at a temperature of 60^0C and a reaction time of 80 minutes.[14] Junior *et al.*, 2018 reported a yield of 65.73% in the transesterification of sunflower oil using K_2CO_3/γ-Al_2O_3 at a reaction time of 240 minutes.[15] However, production processes using biocatalysts of aromatic compounds have never been conducted. In addition to being eco-friendly and cost-effective, the use of this catalyst type eliminates the need for intricate and time-consuming pretreatment typically associated with heterogeneous catalysts. The presence of organic aromatic compounds in biodiesel is not problematic, as these compounds function as antioxidants, thereby enhancing oxidation stability. In the event of separation, it can be achieved easily, typically with the residual methyl acetate at the end of the reaction through co-distillation. The application of biocatalysts comprising aromatic compounds also addresses mass transfer limitations due to the different solubility of the two reactants.

Several studies have explored the production of biodiesel through the interesterification process, using various processes and catalysts. For instance, when interesterification of palm oil with immobilized lipase enzyme was conducted, a 68% yield was achieved at a reaction time of 10 hours.[16] In another study, the reaction between cottonseed oil and methyl acetate, facilitated by ultrasound, yielded a 98.12% conversion. This outcome was obtained at a 1:14.87 molar ratio, 1.17% catalyst concentration, and 67.64% ultrasound amplitude.[17] In the palm oil reaction using ultrasound, the yield was 99.66% at a 1:8.95 molar ratio of oil: methyl acetate, 1.44% catalyst concentration, and 10.03 minutes reaction time.[18] The reaction of palm oil and methyl acetate using the same technique generated a 98.64% yield at a 1:18.74 molar ratio of oil: methyl acetate, 1.24% catalyst concentration, 57.85°C reaction temperature, and 12.69 minutes reaction time.[19] Interesterification of rapeseed oil with methyl formate, conducted at 30°C for 45 minutes, with a molar ratio of oil to methyl formate of 36, and a 1M *t*BuOK catalyst in *t*BuOH, produced a FAME concentration of 93%.[20] Reaction of nyamplung seed oil with ethyl acetate using the lipase enzyme obtained a conversion of 41.46% at 44.43°C, 5 hours reaction time, and 20% enzyme concentration.[21] Interesterification of palm oil with a 0.75% KOH catalyst obtained a yield of 57.30%, at 60°C, 1 hour reaction time, and 300 rpm stirring speed.[8] Using the same ingredients but with 0.5% NaOH catalyst, the reaction temperature of 60°C, 1 hour reaction time, 400 rpm stirring speed, a yield of 87.18% was obtained.[7]

The process of making biodiesel from palm oil has been widely explored. However, the incorporation of biocatalysts with aromatic compounds has never been conducted. This study introduces a novel approach to biodiesel synthesis, aiming for enhanced efficiency by using a catalyst that eliminates the need for a separation process. Aromatic compounds, besides serving as biocatalysts, also function as solvents for reactants and antioxidants. In this report, the compounds used were eugenol and cajuput oil. Eugenol was the main component of clove oil, which, from Gas Chromatography (GC) analysis, constitutes 25.261%.[22] Therefore, this study aimed to determine the optimum conditions for the interesterification process of palm oil with biocatalysts of aromatic compounds. Furthermore, it was conducted to obtain the concept of molecular behavior of aromatic biocatalysts in the interesterification reaction of palm oil into methyl esters.

2. Experimental

2.1. Materials

The materials used in this study were reagents [methyl acetate (Sigma Aldrich, 99.9%) and palm oil (brand Sunco)], catalysts [commercial cajuput oil (brand Gajah) and commercial eugenol] and auxiliary materials [aquadest (H_2O), acetone, potassium hydroxide (Merck, 90%) and phenolphthalein indicator (pp)].

2.2. Methods

2.2.1. Interesterification Reaction with Aromatic Compound Biocatalyst

A total weight of 250 g of palm oil, with a molar ratio of palm oil to methyl acetate set at 1:6, and a biocatalyst of 0.75% wt, were weighed according to the study variables. Palm oil was introduced into a three-neck flask, while a separate Erlenmeyer flask was used for a mixture of methyl acetate and biocatalyst, and then both ingredients were heated to 60^0C. After reaching the desired reaction temperature, the methyl acetate and biocatalyst mixture were combined with the pre-heated palm oil in the three-neck flask using a hot plate. Subsequently, all the components were placed in the three-neck flask, which was equipped with a condenser for reflux, and the reaction temperature was maintained at 60^0C. Stirring was initiated at 300 rpm using a magnetic stirrer, and the calculation of reaction time, namely 15, 30, 45, 60, 75 minutes, commenced in accordance with the specified variables. Upon reaching the designated reaction times, 50 grams of the resulting product were extracted for each corresponding reaction time.

2.2.2. The Process of Separation of Interesterification Reaction Results with Aromatic Compound Biocatalysts

The reaction sample was subjected to distillation at 105^0C to separate the remaining methyl acetate and water from the mixture. Distillation was conducted until no drips of distillate were observed, effectively removing methyl acetate with a boiling point of 57^0C and water with a boiling point of 100^0C. Residues, including oil/triglycerides from the reaction (bp = 383^0C), methyl esters (bp = 373.78^0C), triacetin (bp = 306.74^0C), eugenol (bp = 253.4^0C), or cajuput oil/cineol (bp = 176.4^0C), were weighed as the final product. After completion of the distillation, the residue was analyzed for concentration and composition by Gas Chromatography (GC). The product under optimum conditions was further analyzed according to biodiesel standard (SNI 7182-2015). Finally, the conversion of triglyceride was calculated using Eq. (1):

$$Conversion\ (\%) = \frac{Reacting\ triglycerides\ (mol)}{Initial\ triglycerides\ (mol)} x\ 100\% \quad (1)$$

2.2.3. Analysis

Density Test[23]

The density test comprised weighing an empty pycnometer, introducing methyl ester into the pycnometer, and re-weighing to determine the density of the methyl ester.

Acid Number Test[24]

The acid number test was conducted by making 100 mL of 0.1 N KOH solution, weighing 19-21 ± 0.05 g of biodiesel sample into an Erlenmeyer, adding 100 mL of acetone solvent into a 250 mL Erlenmeyer, and pipetting 3 drops of the PP indicator. Subsequently, the solution was titrated until it turned pink, a colour that lasted for at least 15 seconds.

Analysis of Methyl Esters

Analysis of the composition and concentration of methyl esters using Shimadzu Gas Chromatography (GC).

2.2.4. Molecular Behaviour Simulation with Software ChemDraw Professional 15.0

The molecular behaviour (molecular modelling) of the compounds included in the interesterification reaction, namely triglycerides, methyl acetate and biocatalysts, was determined by simulation using ChemDraw software. Parameters related to the interactions of these compounds can also be calculated using the software. The known molecular behaviour and parameters were the bond distance between atoms before and after the addition of the biocatalyst, potential energy, kinetic energy, and dipole moment.

3. Results and Discussion

3.1. Analysis Results of GC (Gas Chromatography)

Fig. 1 shows the chromatogram of the methyl ester formed via the interesterification reaction of palm oil with cajuput oil biocatalyst at the optimum reaction time of 75 minutes.

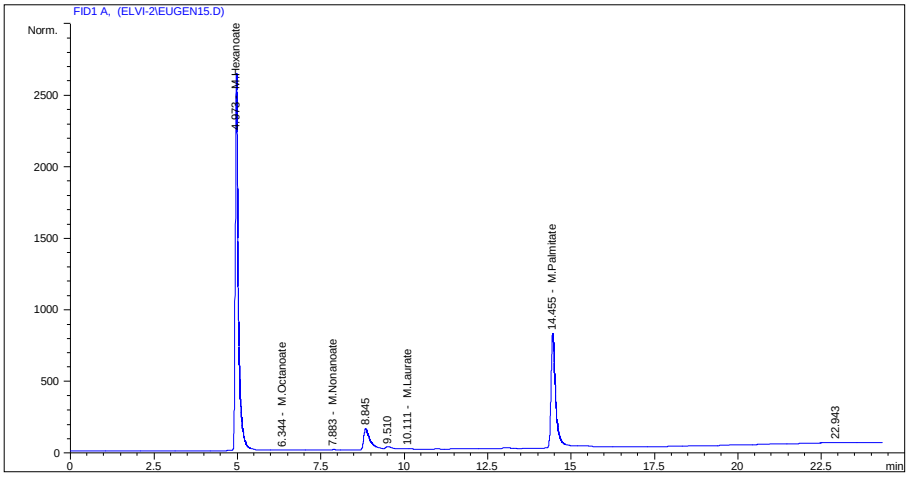

Fig. 1. Chromatogram GC of methyl ester with the addition of cajuput oil biocatalyst at a reaction time of 75 minutes

The FAME composition from palm oil and methyl acetate interesterification reaction using the cajuput oil biocatalyst is shown in Table 1 at 0.75% weight oil, 300 rpm stirring speed, 60^0C reaction temperature, and 75 minutes reaction duration. The main component of FAME is methyl hexanoate, which is a short-chain methyl ester,

formed from the breakdown of methyl linoleate.[25] The breakdown led to the formation of short-chain methyl esters and aldehyde compounds.[26]

Table 1. Composition of FAME results of GC with cajuput oil biocatalyst at 75 min reaction time

FAME (Fatty Acid Methyl Esters)	Formula	Composition (%)
Methyl hexanoate	$C_7H_{14}O_2$	89.3504
Methyl nonanoate	$C_{10}H_{20}O_2$	2.1881
Methyl laurate	$C_{13}H_{26}O_2$	2.9479
Methyl palmitate	$C_{17}H_{34}O_2$	5.5135

3.2. Interesterification Reaction with Aromatic Compound Biocatalyst

Fig. 2 shows that the optimum condition for the eugenol biocatalyst was achieved at a reaction time of 15 minutes, resulting in the highest conversion of triglycerides at 39.4771%. According to Fig. 2, the conversion of the reaction decreased after a reaction time of 15 minutes when the eugenol biocatalyst was applied. This condition was different when the reaction time was varied between 5 and 10 minutes. In the interesterification reaction using the eugenol biocatalyst, the equilibrium was achieved at a reaction time of 15 minutes. Supposing the reaction is reversible, extending the reaction time will favor the equilibrium toward the reactants, consequently diminishing the formation of products.[27] Conversely, with the cajuput oil biocatalyst, the reaction time was observed to be directly proportional to the conversion of triglycerides obtained. During the application of this catalyst, the optimum reaction time was not reached, but the highest conversion of 14.0196% was obtained at 75 minutes. The product of the interesterification reaction with eugenol biocatalyst or cajuput oil was a mixture of methyl ester, triacetin, as well as biocatalyst and unreacted triglycerides. At the reaction time of 30 minutes in the interesterification process with biocatalyst eugenol, there was a decrease in the conversion of triglycerides. This was due to the backreaction of the methyl ester formed, causing the loss of the methyl ester.[28,29] In the interesterification reaction, the stoichiometric molar ratio of palm oil to methyl acetate was theoretically 1:3. However, in this process, a 100% excess of methyl acetate was used, adjusting the ratio to 1:6. This excess is introduced because of the reversible nature of the reaction. According to Le Chatelier's principle, the several means of shifting the equilibrium of a reversible reaction to the right (products) include increasing the reactants, raising the temperature and pressure of the reaction, and separating the products formed.

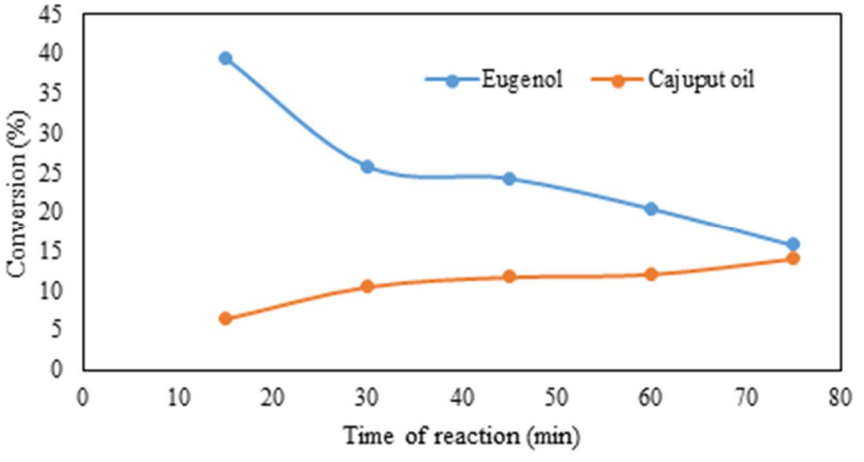

Fig. 2. The correlation between reaction time (min) to conversion (%) with various types of biocatalysts

3.3. Analysis Results of GC-MS (Gas Chromatography-Mass Spectra), Density and Acid Number

Based on the results of GC-MS analysis, the concentration of eugenol ($C_{10}H_{12}O_2$) was 56.645%. Fig. 3 shows the eugenol chromatogram from GC-MS analysis.

Based on the analysis, the concentration of 1,8-cineole ($C_{10}H_{18}O$) in cajuput oil was 29.596%. Fig. 4 shows the 1,8-cineole chromatogram from GC-MS analysis.

Analysis of density and acid number was conducted under the best conditions for each study variable. For the eugenol and cajuput oil biocatalysts, the analysis occurred at a reaction time of 15 and 75 minutes.

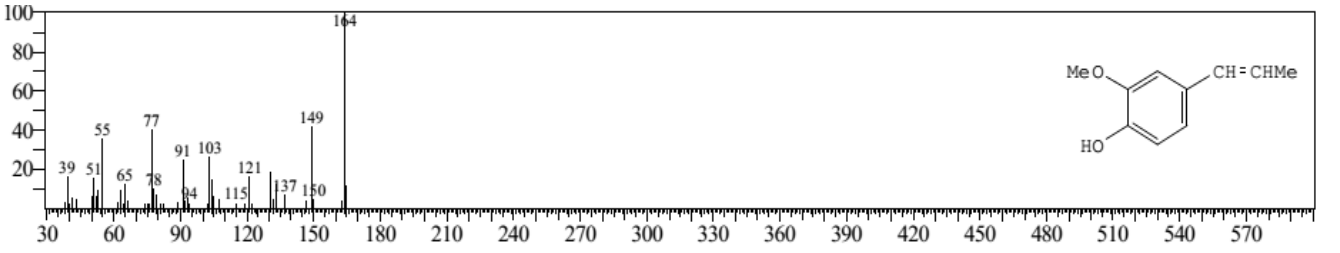

Fig. 3. Chromatogram GC-MS of eugenol

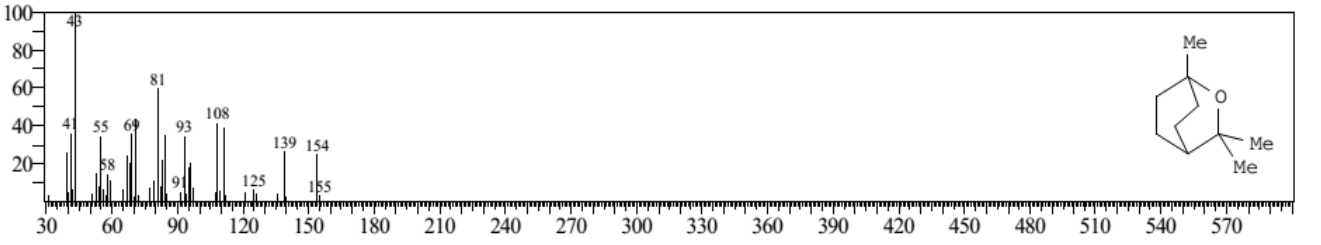

Fig. 4. Chromatogram GC-MS of 1,8-cineole

Table 2. Density and acid number data

Type of biocatalyst	Time of reaction, min	Density, g/mL	Acid number, mg KOH/g
Eugenol	15	0.892	0.337
Cajuput oil	75	0.908	0.426

Table 2 shows that all acid numbers in the interesterification process using eugenol and cajuput oil biocatalysts met the standard SNI 7182:2015, with the maximum value being 0.5 mg KOH/g. A lower acid number is desirable as it indicates a reduced formation of free fatty acids in the product. The dual functionality of eugenol and cajuput oil, acting not only as biocatalysts but also as antioxidants, plays a crucial role in preventing oxidation reactions and the consequent generation of free fatty acids. Meanwhile, in the same process, all density values did not meet the SNI 7182:2015 standard of 0.85-0.89 g/mL. This is because the reaction product is a mixture of methyl ester, triacetin, as well as residual triglycerides and biocatalyst. It is important to note that the biocatalyst was not separated. The density obtained was the average of the four components in the reaction product.

3.4. Molecular Behaviour Simulation with ChemDraw Professional Software 15.0

Under the influence of a magnetic field, the oxygen (O) atom undergoes an attractive force, leading to a noticeable difference in the distance between the O atom and the magnetic field. This variation in distance is evident in both Fig. 5 and Fig. 6, representing the state of the system before and after magnetic field induction, specifically in the context of aromatic compounds.

Fig. 5 shows the difference in the distance between the O atoms in triglycerides and methyl acetate, as well as the aromatic/aryl groups in eugenol (C_{76}). The distance between the C_{76} and the O_{13} atoms (R_1 in the triglyceride) changed from 10,741Å to 10.724Å. This shows that the O atom with 2 free electrons had paramagnetic behavior, being drawn towards the magnetic field associated with the aromatic group of eugenol. A similar observation was noted in the O_{15} atom (R_2 in triglycerides), where the distance from the C_{76} atom changes from 11.237Å to 11.203Å. The distance between the C_{76} and the O_{74} atom (R in methyl acetate) changed from 23.533Å to 23.403Å, a reduction of 0.13Å. The influence of the magnetic field on the O atom weakens the bond between the adjacent C atoms and the O atom.

Fig. 6 provides a visual representation of the distance between the O atoms in triglycerides and methyl acetate, as well as the aromatic/aryl groups in cineol (C_{76}). The distance between the C_{76} and the O_{13} atom (R_1 in the triglyceride) changed from 10.028Å to 10.014Å, a reduction of 0.014Å. At the O15 atom (R_2 in triglycerides), the distance from the C_{76} atom changed from 9.502Å to 9.466Å. Between the C_{76} atom and the O_{74} atom (R in methyl acetate), it shifted from 21.622Å to 21.519Å, a reduction of 0.103Å is less. The influence of the magnetic field on the O atom weakened the bond between the adjacent C and the O atom.

In triglycerides and methyl acetate, the C─O and C═O groups had polarity due to dipole moments. These groups strongly bind the non-polar R (alkyl) group to triglycerides and methyl acetate through van der Waals

forces (dipole-dipole interactions). The C=O group, with greater electronegativity, was particularly responsive to magnetic fields.[30] Organic aromatic compounds like eugenol and cineol generated a magnetic field due to the delocalization of electrons in the aromatic structures.[31,32] When the C=O group was in proximity to a compound, the van der Waals force between the molecule and the carbon chain weakened.[31] The combination of this force with added energy (e.g., heat energy) results in the breaking of the R bond. The C─C bond, with a low bond energy of 347 kJ/mol, was the first to break. The breaking of the R group on triglycerides and methyl acetate triggers a substitution reaction where positions are being exchanged, following the interesterification reaction mechanism.

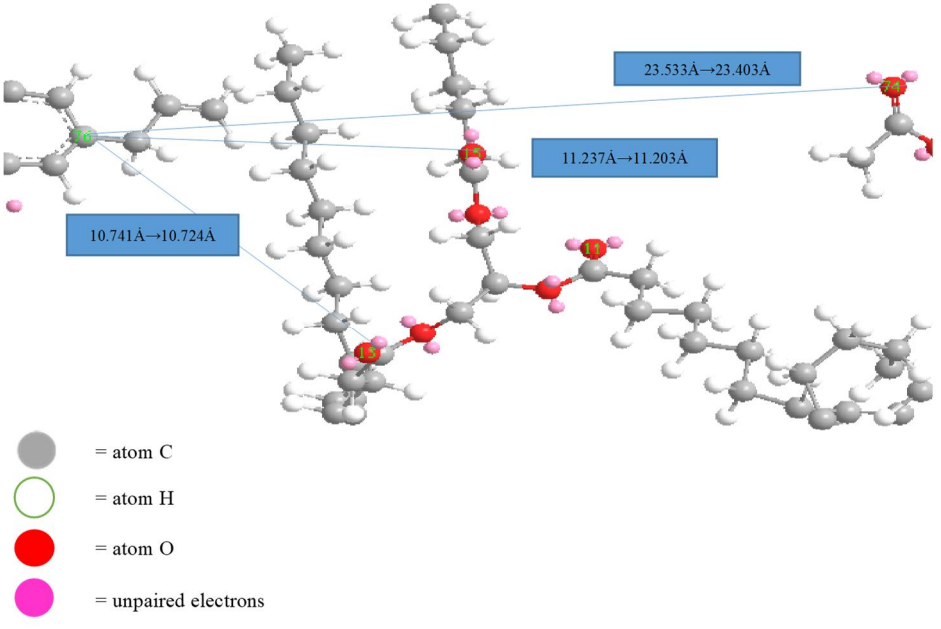

Fig. 5. The distance of the O atom in triglycerides and methyl acetate to the C atom in eugenol

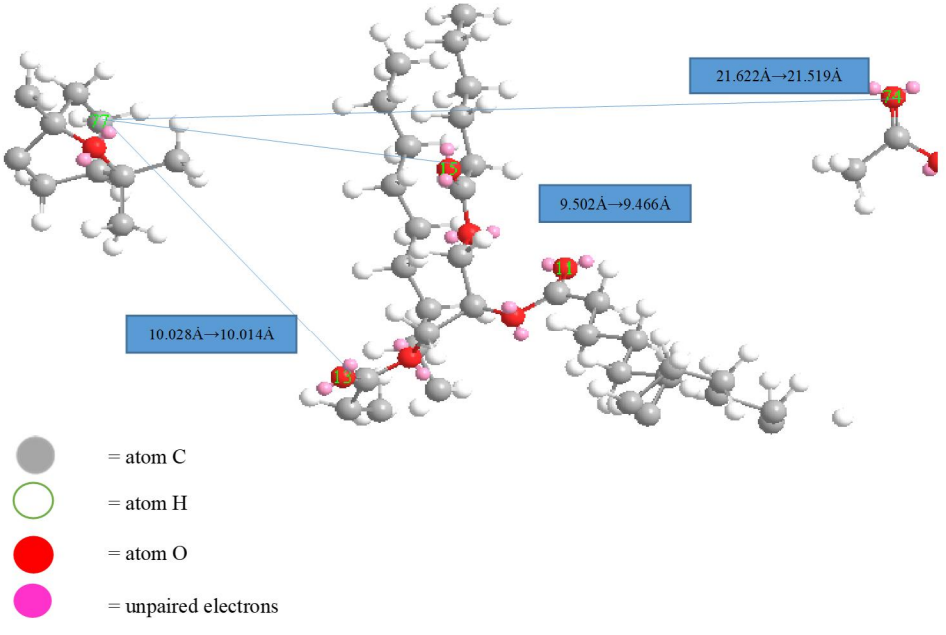

Fig. 6. Distance of O atoms in triglycerides and methyl acetate to C atoms in cineol (cajuput oil)

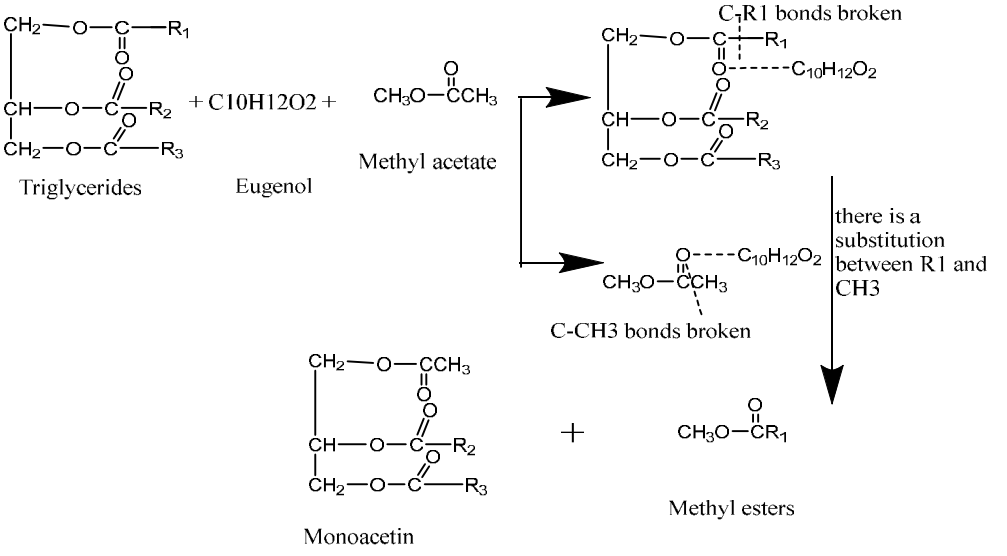

Fig. 7. Interesterification reaction mechanism of triglycerides and methyl acetate with eugenol biocatalyst to form monoacetin and methyl esters

3.5. Calculation of kinetic energy and potential energy with software ChemDraw Professional 15.0

Table 3 showed that the addition of biocatalysts of aromatic compounds enhanced the reactivity of the reactants, namely, triglycerides and methyl acetate, compared to those without biocatalysts. This was observed from the initial kinetic energy value of the reactants, which increased from 2914.6673 kJ/mol to 3445.6577 kJ/mol after the addition of eugenol. The incorporation of this biocatalyst to triglyceride and methyl acetate made the components more mobile than when cineol was added. This was indicated by higher kinetic energy and the average C-C bond length, which is greater than cineol. Higher kinetic energy implies more active movement of the components,[33] making it the most influential factor for the stability of a molecule. A higher value of this energy indicates an increased instability, making it easier for electrons to transition from the valence to the conduction band.

From Table 3, it was evident that the addition of biocatalysts of aromatic compounds produces a greater dipole moment. The initial dipole moment of the reactants was 3.9504 debyes, but after including eugenol as a catalyst, the value increased to 4.7175 debyes. Based on the calculation, cineol produces a greater dipole moment than eugenol. Consequently, triglycerides and methyl acetate had more solubility with the addition of cineol. The greater the value of the dipole moment, the higher the molecular interactions within the components.[34] This proves that aromatic compounds, besides their role as biocatalysts, also serve as solvents for reactants.

Table 3. Calculation of kinetic energy and dipole moment on components using ChemDraw

Component	E Potential, kJ/mol	E Kinetic, kJ/mol	Dipole Moment, debye
Triglicerides + methyl acetate + eugenol	-6895.0140	3445.6577	4.7175
Triglicerides + methyl acetate + cineol	-6754.7527	3376.2807	5.3944
Triglicerides + methyl acetate	-5832.3952	2914.6673	3.9504

According to Fig. 2, which shows the relationship between reaction time (minutes) and conversions FAME (%), the application of cajuput oil (cineol) biocatalyst requires an extended duration to produce high yields. This is because the concentration of cineol in commercial cajuput oil is small, at 28.84%.[35] The interesterification process is affected by the limited solubility of triglycerides and methyl acetate due to their constrained concentration. On the contrary, employing

ChemDraw for simulation to ascertain the dipole moment using the cineol parameter set at 100%, reveals that the eugenol biocatalyst, with a concentration of 56.645%, has a significant solubility in both triglycerides and methyl acetate.

4. Conclusions

1. Eugenol was the most effective catalyst in the palm oil interesterification process compared to cajuput oil. The results showed that the optimum conditions for the palm oil interesterification process with eugenol biocatalyst were 0.75% oil mass, 15 minutes reaction time, 1:6 molar ratio of palm oil to methyl acetate, 60°C reaction temperature, and 300 rpm stirring speed. Under these conditions, the conversion, density, and acid number were 39.4771%, 0.892 g/mL, and 0.3 mg KOH/g sample, respectively.

2. The simulation using ChemDraw software further showed that the application of eugenol induced the movement of the most reactive triglycerides and methyl acetate molecules. Simulation results from ChemDraw Professional 15.0 showed that the use of eugenol biocatalyst induced the most significant change in the O atomic distance in triglycerides and methyl acetate, with C atoms in eugenol compared to other biocatalysts.

3. The kinetic energy with the eugenol biocatalyst attained a value of 3445.6577 kJ/mol, surpassing the observed value with the cineol biocatalyst (cajuput oil). Aromatic compounds, besides their role as biocatalysts, also function as reactant solvents. This is evident from the simulation results showing a change in the dipole moment from 3.9504 debyes to 5.3944 debyes after the addition of cajuput oil biocatalyst.

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ДОСЛІДЖЕННЯ ПРОЦЕСУ ПЕРЕЕСТЕРИФІКАЦІЇ ПАЛЬМОВОЇ ОЛІЇ В МЕТИЛОВІ ЕСТЕРИ ЗА ДОПОМОГОЮ БІОКАТАЛІЗАТОРІВ АРОМАТИЧНИХ СПОЛУК

Анотація. *Реакцію переестерифікації пальмової олії та метилацетату для отримання метилового естеру та триацетину проводили з біокаталізаторами ароматичних сполук, а саме евгенолу та каяпутової олії. Ароматичні сполуки є найефективнішими каталізаторами в процесі виробництва біодизелю, що приводить до покращення якості. Тому це дослідження мало на меті отримати ефективніший і результативніший процес виробництва біодизелю з меншою кількістю процедурних етапів для зниження виробничих витрат. Робочі умови дослідження включали масу пальмової олії 250 г, молярне співвідношення пальмової олії до метилацетату 1:6, температуру реакції 60°C, швидкість перемішування 300 об/хв, масу каталізатора 0,75% від маси пальмової олії, а також час реакції 15, 30, 45, 60 і 75 хвилин. Молекулярна поведінка та параметри, такі як відстань зв'язку між атомами до та після додавання біокаталізатора, потенційна енергія, кінетична енергія та дипольний момент, були визначені за допомогою моделювання з використанням програмного забезпечення ChemDraw.*

Ключові слова: *переестерифікація, ароматичні сполуки, каталізатор, кінетична енергія, дипольний момент.*