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Fajar, Rizqon

Research Center for Transportation Technology, National Research and Innovation Agency

Ma' ruf, Muhammad

Research Center for Energy Conversion & Conservation Technology, National Research and Innovation Agency

Yubaidah, Siti

Research Center for Energy Conversion & Conservation Technology, National Research and Innovation Agency

Nurfadillah, Agung

Laboratory for Thermodynamics, Motor & Propulsion, National Research and Innovation Agency

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Optimizing Palm-Based Bio-lubricant Formulations for Diesel Engine Using Machine Learning and Experimental Techniques

Rizqon Fajar^{1,*}, Muhammad Ma'ruf², Siti Yubaidah², Agung Nurfadillah³

¹Research Center for Transportation Technology, National Research and Innovation Agency, South Tangerang, 15314, Indonesia

²Research Center for Energy Conversion & Conservation Technology, National Research and Innovation Agency, South Tangerang, 15314, Indonesia

³Laboratory for Thermodynamics, Motor & Propulsion, National Research and Innovation Agency, South Tangerang, 15314, Indonesia

*Author to whom correspondence should be addressed:

E-mail: rizqon.fajar@brin.go.id

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Abstract: Integrating bio-lubricants into internal combustion engines is crucial for sustainable engineering, driven by the need for renewable and eco-friendly alternatives. However, bio-lubricants in diesel engines often face challenges related to insufficient thermal-oxidative stability. This research introduces a novel approach to enhance the thermal-oxidative stability and lubricity of palm oil-derived bio-lubricants for diesel engine applications. By chemically modifying palm olein through transesterification, epoxidation, and oxirane ring-opening, and leveraging the predictive capabilities of the 'BimolP' machine learning tool, we identified base stocks with improved properties. Our results show significant enhancements in thermal-oxidative stability, with the decomposition onset temperatures (T_{onset}) of modified palm olein increasing from 280°C to 281°C and 295°C, and those of palm methyl ester derivatives rising from 222°C to 245°C and 268°C. Additionally, the friction coefficient of palm olein derivatives increased from 0.104 to 0.106 and 0.113, and for methyl ester derivatives, it rose from 0.101 to 0.108 and 0.113. The final bio-lubricant formulation combines various modified base stocks to meet SAE-30 and SAE-40 diesel lubricant specifications. This study underscores the effectiveness of integrating chemical modifications, machine learning predictions, and blending palm-based stocks to optimize bio-lubricant formulations without the need for prior synthesis or modification of palm olein and palm methyl ester.

Keywords: bio-lubricant; thermal-oxidative stability; lubricity; viscosity; trans-esterification; epoxidation; ring-opening

1. Introduction

The pressing need to address climate change and pollution, particularly in the transportation and industrial sectors, mandates reducing greenhouse gas emissions. Bio-lubricants derived from palm oil emerge as a promising solution to mitigate the environmental impact of traditional lubricants. The renewable nature of palm oil has the potential to substantially decrease the carbon footprint in both the production and application of lubricants, offering a solution to environmental challenges such as oil spills. Integrating palm bio-lubricant into combustion engines will reduce CO, HC and smoke emissions and improve engine efficiency¹⁾. Nevertheless, a significant challenge lies in optimizing the thermal-oxidative stability of these bio-lubricants while preserving

their high lubricity properties. This delicate balance is essential to ensure bio-lubricant efficacy in demanding diesel engine environments, where elevated temperatures and pressures may compromise their chemical integrity. Therefore, careful chemical modifications to enhance thermal-oxidative stability are imperative to guarantee the reliability of bio-lubricants^{2,3)}.

Incorporating palm bio-lubricants into diesel engines faces challenges due to the stringent thermal-oxidative stability and lubricity requirements of these engines. Biodiesel as a fuel directly interacts with the bio-lubricant in the engine combustion chamber, impacting lubricant viscosity and, consequently, its service life. Successfully addressing these challenges is vital for effectively integrating palm bio-lubricants into diesel engines, contributing to sustainable and eco-friendly transportation

solutions. Diesel engines necessitate lubricants with robust thermal-oxidative stability to withstand high temperatures and pressures during operation, as inadequate thermal-oxidative stability can lead to increased oxidation, wear, reduced lubricity, and the formation of engine deposits. Overcoming these challenges is crucial for successful integration, requiring formulation advancements to enhance thermal-oxidative stability while maintaining other essential properties. This ensures optimal engine performance, minimizes wear, and mitigates the risk of deposits, contributing to the longevity and efficiency of diesel engines⁴⁾.

Addressing the critical challenge of improving the thermal-oxidative stability of palm-based bio-lubricants for diesel engines is essential. The interaction between biodiesel fuel and bio-lubricants in the combustion chamber further complicates this by affecting viscosity and shortening service life. Therefore, it is vital to develop bio-lubricant formulations that enhance thermal-oxidative stability while maintaining excellent lubricity.

This study introduces innovative formulations of high-performance palm-based bio-lubricants with enhanced thermal-oxidative stability and lubricity for diesel engines. By employing chemical modifications such as transesterification, epoxidation, and ring structure opening of palm oil derivatives, combined with machine learning techniques for optimization, it pioneers the development of bio-lubricant blends from various modified palm oil derivatives that meet SAE-30 and SAE-40 viscosity specifications. These novel formulations, specifically the unique combinations of two- and three-base stocks, have not been previously explored, positioning this research at the forefront of sustainable and eco-friendly lubricant development.

2. Literature Review

2.1. Impact of Thermal-oxidative Stability, Lubricity, and Viscosity of Bio-Lubricants on Diesel Engine

Bio-lubricants are emerging as a promising alternative to conventional mineral lubricants, offering significant benefits in terms of thermal-oxidative stability, lubricity, and viscosity.

Table 1. Review of the impact of thermal-oxidative stability, lubricity & viscosity

Reference	Bio-lubricant Formulation	Effect on Diesel Engine
Arumugam et al. (2014) ⁵⁾	Modification of rapeseed oil through epoxidation, ring-opening, esterification, and addition of anti-wear additive	Enhanced lubricity and thermal-oxidative stability in rapeseed oil bio-lubricant, along with an anti-wear nano CuO additive for improved

		viscosity, reduce engine wear and extend engine service life.
Dey & Misra (2017) ⁶⁾	Pure palm Oil	Palm biodiesel bio-lubricants enhance oxidative stability and lubricity, reducing engine deposits and wear
Cahyono et al. (2021) ⁷⁾	Modification of castor oil through esterification, transesterification, epoxidation, and ring-opening reaction	Bio-lubricants can reduce engine wear compared to mineral lubricants but may experience oxidation and viscosity changes, leading to thickening, sludge formation, and deposits
Tasneem et al. (2022) ⁸⁾	A mixture of Karanja methyl ester (KME) and mineral oil	A blend of bio-lubricants & mineral lubricants enhances oxidative stability and lubricity, reducing engine deposits and wear.
S.G. Muthurathinam & A.V. Perumal (2023) ⁹⁾	Methyl esters of Neem, Pongamia & Tamanu Oils	Bio-lubricants, with their superior oxidative stability, enhanced lubricity through chemical modifications, and favourable viscosity characteristics, reduce engine deposits and wear.

Modifying rapeseed oil through processes such as epoxidation, ring-opening, esterification, and the addition of an anti-wear nano CuO additive enhances both lubricity and thermal-oxidative stability⁵⁾. This comprehensive modification reduces engine wear and improves viscosity, resulting in an extended engine service life. Similarly, the bio-lubricant of a mixture of Karanja methyl ester and mineral lubricant offers improved oxidative stability and lubricity, which are crucial for reducing engine deposits and wear. Maintaining proper viscosity ensures adequate lubrication, further extending the engine's service life and ensuring reliable performance.

However, while bio-lubricants show potential, they also present challenges that need to be addressed. Pure palm

oil-based bio-lubricants enhance oxidative stability and lubricity, reducing engine deposits and wear. Nonetheless, variations in viscosity and density during engine operation can influence overall performance and emissions. The infiltration of the lubricant into the fuel side can further affect engine wear and service life. Additionally, bio-lubricants derived from castor oil through esterification, transesterification, epoxidation, and ring-opening reactions can reduce engine wear compared to mineral lubricants. However, these bio-lubricants may experience oxidation and viscosity changes, leading to thickening and sludge formation, which can cause deposits and negatively impact engine performance and longevity. Therefore, while bio-lubricants offer significant advantages, their formulation and application must be carefully optimized to maximize benefits and minimize potential drawbacks.

In summary, bio-lubricants from vegetable oils and their derivatives positively impact diesel engine performance due to their superior lubricating properties compared to mineral lubricants. However, the long-term effects on components and lubricant lifespan need further investigation, especially regarding variations in the mixture of different raw materials and chemical structural modifications to enhance thermal-oxidative stability¹⁰. It is essential to control oxidation at high temperatures and prevent sludge deposits on engine components, which could potentially cause engine damage. Optimizing the blending composition between pure plant oil, methyl ester, and other vegetable oil derivatives is necessary to produce a bio-lubricant with high thermal-oxidative stability. Bio-lubricants must be mixed with mineral oil to protect the engine from wear or damage¹¹. This is because commercial mineral lubricants contain various additives that protect the engine, such as anti-wear, anti-oxidant, extreme pressure, and detergents¹².

2.2. Enhancing Thermal-oxidative Stability and Lubricity of Palm Bio-lubricant

Table 2 presents various chemical modification approaches to vegetable oil, including esterification/transesterification, hydrogenation, epoxidation, and estolide formation. Generally, all these chemical modifications are carried out to reduce double bonds or transform one type of ester into another with higher thermal-oxidative stability. For use as a bio-lubricant base stock in diesel engines, an enhancement of thermal-oxidative stability is required¹³ due to the high temperatures and pressures in the combustion chamber of an operating diesel engine (which can exceed $>1500^{\circ}\text{C}$ and $>10\text{MPa}$). Two chemical modification approaches meet these criteria through epoxidation and estolide formation reactions. These chemical modifications improve the lubricity, thermal-oxidative stability, and the pour point, making them advantageous in terms of ease and cost of operation, especially epoxidation. Estolide formation is highly undesirable due to its high production

cost. The improvement of the pour point after epoxidation can be addressed by further reactions, such as ring-opening, to form branched chains¹⁴.

Table 2. Chemical modifications of vegetable oil²

Chemical Modification	Advantages	Disadvantages
Esterification / Trans-esterification	- Improves thermal-oxidative stability - Improves low-temperature properties	- Requires feedstock with high oleic acid content - High reaction temperature
Selective hydrogenation	- Reduces degree of unsaturation - Improve oxidative stability	- isomerization reactions (cis-and tram-acids) - High reaction temperature
Epoxidation	- Improves lubricity - Improves thermo-oxidative stability - Low-reaction temperature	- Increases pour point value - Decreases viscosity index
Estolide formation	- Improves thermo-oxidative stability - Low reaction temperature - Allows the use of several vegetable oils	High production cost

Chemical modification through esterification/transesterification can enhance thermo-oxidative stability and low-temperature flow properties. However, the drawback is that it requires feedstock with a high oleic acid content, and the reaction occurs at high temperatures. On the other hand, modification through hydrogenation, aside from requiring high reaction temperatures, results in the isomerization of cis- and trans-acids and reduces bio-lubricant fluidity, forming solids or waxes. Hydrogenation of double bonds is considered ineffective in improving the key properties of bio-lubricants.

2.3. Prediction of Thermal-oxidative Stability and Lubricity Using Machine Learning

In the design or formulation phase, predicting the onset temperature of decomposition (T_{onset}) and lubricity (coefficient of friction, CoF) of the base stock compounds in a bio-lubricant is crucial. Therefore, there is no need to synthesize base stock compounds beforehand, and

measurements of T_{onset} and CoF are also unnecessary, as this will save time and costs. T_{onset} and CoF of the selected base stocks and mixtures will be validated through measurements. The mixture with the best properties will be tested on a diesel engine. Predictions for thermal decomposition and tribological properties are made by establishing a correlation between a descriptor providing structural information and the key properties of the base stock compounds under investigation (T_{onset} and CoF)^{15,16}.

There are four stages in predicting T_{onset} and CoF using machine learning:

1. Chemical Compound Data Collection Stage: Collecting chemical compound data from palm oil derivatives by gathering experimental data from literature and previous research.
2. Structure and Descriptor Data Collection Stage (using software): Software tools collect structural and descriptor data.
3. Data Pre-processing and Modeling Stage involves data pre-processing and the actual modelling process.
4. Model Validation and Optimization Stage: The model undergoes validation and optimization in this final stage.

3. Methodology

3.1. Preparation and Selection of Base Stock Used for Bio-lubricant Formulation

Based on the results of a review of various literature^{2,3,14,17–21}, the base stock for bio-lubricant formulation will be derived from palm olein, palm methyl ester, and its derivatives through epoxidation and ring-opening reactions. Compounds used as reactants in the ring-opening reaction include methyl and ethyl amine. The procedures employed in the epoxidation and ring-opening reactions follow references¹⁴. The palm olein used in this research is commercial palm oil obtained from the local market, and methyl ester purchased from a local biodiesel plant in Indonesia.

Several potential base stocks for diesel engine bio-lubricant formulations have been identified, including palm olein (PO)^{22,23}, palm methyl ester (PME)²⁴, epoxidised palm olein (EPO)^{25–27}, epoxidised palm methyl ester (EPME)²⁸, ring-opened epoxidised palm olein (Palm Olein Hydroxy Methyl Amine), and ring-opened epoxidised palm methyl ester (Palm Methyl Ester Hydroxy Methyl Amine). The thermal-oxidative stability (T_{onset}) and lubricity properties (CoF) of these base stocks will be predicted using machine learning techniques to guide the selection process for formulation. This selection will focus on developing bio-lubricant formulations from various base stock combinations.

3.2. Modeling Key-Properties of Base Stock Using Machine Learning

The key properties predicted using machine learning techniques are T_{onset} and Coefficient of Friction (CoF),

which are crucial in determining bio-lubricant formulations^{29,30}. On the other hand, viscosity, viscosity index, and pour point can be easily obtained from the literature³¹. If measured, they are also relatively quick and cost-effective¹⁷.

Prediction of onset temperature and coefficient of friction for pure compounds were made using the BimolP: Bio-lubricant Molecule Properties Analyzer³². This program was developed using Python³³ and utilizes the main library called Mordred³⁴ to calculate molecular descriptors. BimolP utilizes machine learning techniques to predict the properties of lubricants based on the molecular structure input, which is provided in SMILES format. The model for the onset temperature prediction has a coefficient of determination (R^2) of 0.884 and a root mean square of error (RMSE) of 17.0 °C, while the coefficient of friction model has an R^2 of 0.894 and an RMSE of 0.10³³.

3.3 Blending Relations for Base Stocks

Strategies are performed by blending two or three base stock components to achieve the target viscosity according to SAE-30³⁵ and SAE-40³⁵. The viscosity and viscosity index measurements were conducted using an Anton Paar SVM 3000 viscometer with the ASTM D445³⁶ and ASTM D2270 methods³⁷. A binary and ternary chart is developed to determine the base oil composition that achieves the target viscosity through calculations. The viscosity calculation of binary/ternary base oil mixture at various composition variations is performed using the following equation:

$$\ln(\eta_{\text{mixture}}) = X_A \cdot \ln(\eta_A) + X_B \cdot \ln(\eta_B) + X_C \cdot \ln(\eta_C)$$

Note: X denotes the weight fraction of each component (A, B, C) in the mixture, and η denotes the viscosity of each component. This equation follows the general form of a viscosity model for mixtures, assuming no interaction parameters exist between components³⁸.

3.4. Characterization and Evaluation of Base Stock Properties

Tables 3 and 4 show data on the molecular weight, viscosity at 100°C, predicted decomposition onset temperature (T_{onset}), and predicted coefficient of friction (CoF) for various palm oil-based molecules: Palm Olein (PO), Epoxidized Palm Olein (EPO), Palm Olein Hydroxy Methyl Amine (POHMA), Palm Methyl Ester (PME), Epoxidized Palm Methyl Ester (EPME), and Palm Methyl Ester Hydroxy Methyl Amine (PMEHMA). Generally, higher molecular weight correlates with higher viscosity due to increased molecular interactions. For example, PO and its derivatives typically have higher viscosities. However, some higher molecular weight molecules, like PMEHEMA compared to PME and EPME, show lower viscosities due to more streamlined structures. This is also seen in the epoxidation and ring opening of palm oil.

Table 3. The molecular weight and viscosity of palm base stocks

Molecule Name	Molecule Formula	Molecule Weight	Viscosity at 100°C (mm ² /s)
Palm Olein	C ₅₅ H ₁₀₂ O ₆	859.42	8.44
Epoxidized-Palm Olein	C ₅₅ H ₁₀₂ O ₈	891.41	13.29
Palm Olein Hydroxy Methyl Amine	C ₅₇ H ₁₁₂ N ₂ O ₈	953.84	18.36
Palm Methyl Ester	C ₁₉ H ₃₆ O ₂	296.50	1.75
Epoxidized Palm Methyl Ester	C ₁₉ H ₃₆ O ₃	312.49	4.61
Palm Methyl Ester Hydroxy Methyl Amine	C ₂₀ H ₄₁ NO ₃	343.55	1.12

Table 4. Predicted onset temperature of decomposition (T_{onset}) and predicted coefficient of friction (CoF)

Molecule Name	Molecule Formula	Predicted T _{onset} (°C)	Predicted CoF
Palm Olein	C ₅₅ H ₁₀₂ O ₆	280.47	0.104
Epoxidized-Palm Olein	C ₅₅ H ₁₀₂ O ₈	294.85	0.106
Palm Olein Hydroxy Methyl Amine	C ₅₇ H ₁₁₂ N ₂ O ₈	281.18	0.113
Palm Methyl Ester	C ₁₉ H ₃₆ O ₂	222	0.101
Epoxidized Palm Methyl Ester	C ₁₉ H ₃₆ O ₃	245.45	0.108
Palm Methyl Ester Hydroxy Methyl Amine	C ₂₀ H ₄₁ NO ₃	268.11	0.113

There is no straightforward correlation between molecular weight versus predicted T_{onset} and CoF. While molecular weight can influence thermal-oxidative stability, other factors, such as molecular structure and functional groups, play a significant role^{2,39}. For instance, Epoxidized-Palm Olein has a slightly higher T_{onset} than Palm Olein, even though it has a similar molecular weight. The coefficient of friction depends on the molecular structure and interactions at the sliding interfaces. The variations in CoF among the molecules may be attributed to differences in functional groups and molecular arrangements. Ester groups contribute more to reducing CoF than epoxide, hydroxyl, and amine groups.

3.5. Formulation and Evaluation of Bio-lubricants

Drawing upon the outcomes of performance and endurance assessments conducted on diesel engines,

along with the measurements and predictions of T_{onset} and CoF, we are equipped to devise formulations for bio-lubricants. Such formulations inherently involve a combination of diverse base stocks, each possessing distinct merits in viscosity, thermal-oxidative stability, and lubricity. Optimization during the formulation process will entail manipulating the composition and cost as control variables, with the performance of the bio-lubricant serving as the targeted variable. There are several possible combinations of base stock mixtures to form bio-lubricant formulations, as listed in Table 5, based on viscosity to meet diesel engine specifications, namely SAE 30 and SAE 40.

Table 5. Options for bio-lubricant composition from various base stock

Base Stock	A mixture of 2 Base Stock	A mixture of 3 Base Stock
Palm Olein	PO+EPO	PO+PME+EPO
Epoxidized-Palm Olein	PO+POHMA PO+PME	PO+PME+POHMA PO+PME+EPME
Palm Olein Hydroxy Methyl Amine	PO+EPME PO+PAMEHMA EPO+PME EPO+EPME EPO+PMEHMA	PO+PME+PMEHMA
Palm Methyl Ester		
Epoxidized Palm Methyl Ester		
Palm Methyl Ester Hydroxy Methyl Amine		

Various mixtures of two- and three-base stocks will be analyzed for viscosity to meet SAE-30 and SAE-40 specifications. T_{onset} and CoF of the selected base stocks and mixtures will be validated through measurements. The mixture with the best properties will be tested on a diesel engine. The bio-lubricant formulated will be tested on non-automotive diesel engines using SAE-30 and SAE-40 lubricants, which are preferred in tropical countries like Indonesia for their thermal-oxidative stability and wear protection under high temperatures and heavy-duty conditions.

4. Results and Discussion

4.1. Key-Properties of Base Stock for Bio-lubricant

The data of the molecular weight, viscosity, thermal-oxidative stability, and coefficient of friction for various palm oil-derived base stocks are summarized in Tables 3 and 4. We observed that higher molecular weights generally correlated with higher viscosities, the expected behaviour of larger molecules exhibiting increased

molecular interactions and entanglements. Sometimes, a molecule with a higher molecular weight can have a lower viscosity than a counterpart with a lower molecular weight. This happens when the molecular structure creates a less entangled configuration, allowing more effortless flow¹⁸⁾. However, exceptions were noted where molecular structure led to streamlined configurations, resulting in lower viscosities despite higher molecular weights. For example, PMEHMA has a higher molecular weight than PME and EPME but exhibits lower viscosity. This phenomenon is also observed in the epoxidation process and ring opening of palm oil¹⁵⁾.

Thermal-oxidative stability, as indicated by T_{onset} , and the coefficient of friction (CoF) were also analyzed. The predicted T_{onset} did not always correlate straightforwardly with molecular weight, indicating that molecular structure and functional groups significantly impact thermal-oxidative stability. For instance, EPO showed a higher T_{onset} compared to PO, even though they have similar molecular weights. The CoF variations among the molecules are attributed to differences in functional groups, with ester groups contributing more effectively to reducing friction compared to epoxide, hydroxyl, and amine groups. The presence of saturated fatty acids in palm oil allows for the formation of a protective layer, resulting in a lower coefficient of friction compared to oils with more unsaturated fatty acids. Consequently, palm fatty acid esters exhibit promising performance characteristics and environmental benefits, making them a competitive choice as a blending component for bio-lubricant formulation, alongside fatty acid esters derived from other vegetable oils^{41,42)}.

This comprehensive analysis underscores the need to balance these properties to optimize bio-lubricant performance. High-viscosity bio-lubricants usually provide better thermal-oxidative stability and lower friction, but the presence of functional groups can modify these relationships. For instance, Epoxidized Palm Methyl Ester, despite having a higher viscosity, shows a higher CoF due to the epoxy group. Similarly, Palm Methyl Ester Hydroxy Methyl Amine, with its hydroxyl group, has a higher CoF despite lower viscosity. Therefore, achieving optimal bio-lubricant performance involves a careful trade-off between molecular weight, viscosity, functional groups, and their impact on T_{onset} and CoF.

4.2. Viscosity Mapping of SAE 30 and SAE 40 of Bio-lubricant Mixtures

Figure 1 shows the viscosity mapping of the mixing results of three base stocks, namely PO, EPO, and EPME, that meet and do not meet the specifications of SAE 30 (A) and SAE 40 (B). For the specifications of diesel engine lubricants with SAE 30, the compositions that meet the criteria are marked with circles (OK); for example, a bio-lubricant formulation that meets SAE 30 is a mixture of PO: EPO: EPME = 0.5: 0.3: 0.2. Meanwhile, the compositions that meet the criteria for SAE-40 are bio-

lubricant formulations with a mixture of PO: EPO: EPME = 0.1: 0.9: 0. The different ratios of PO, EPO, and EPME indicate how varying each component affects the overall viscosity. EPO, with its higher intrinsic viscosity, plays a crucial role in reaching the required viscosity for SAE 40. Thus, with simulations like this, we can choose the composition of mixtures that satisfy the viscosity specifications of SAE-30 and SAE-40 for a specific diesel engine. The ability to map and predict the viscosities of bio-lubricant mixtures is crucial for formulating products that meet industry standards. The mixtures that meet SAE 30 are typically suitable for lighter engine loads and moderate temperatures, while those meeting SAE 40 can handle higher loads and temperatures more effectively.

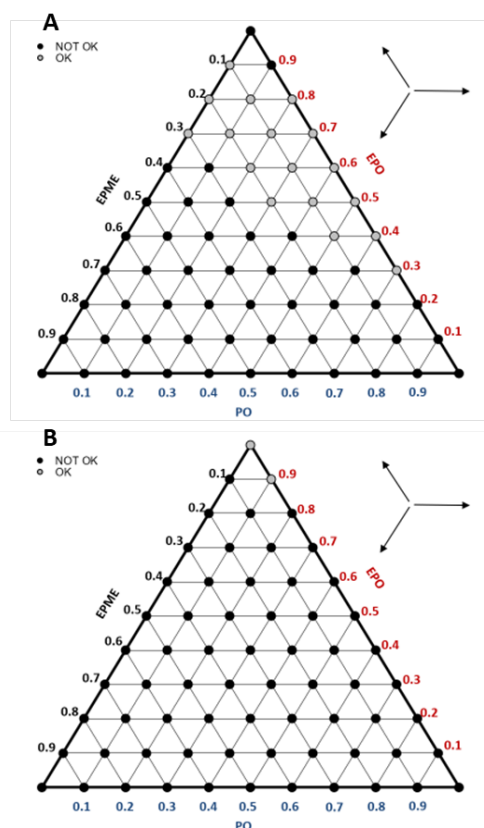


Fig. 1: The Viscosity map for mixtures of three base stocks (PO, EPO & EPME) for SAE-30 (A) and SAE-40 (B)

In addition to three-base stock mixtures, we also explored the viscosity mapping of mixtures consisting of two base stocks, as seen in Fig.2. Fig.2(A). and Fig.2(B). show the viscosity mappings for PO and EPO mixtures for SAE 30 and SAE 40, respectively. These mappings provide insights into the minimum required proportions of each component to meet the viscosity standards.

These viscosity mappings serve as a guide for selecting and blending base stocks to formulate bio-lubricants that not only meet the required specifications but also offer enhanced performance characteristics such as improved thermal-oxidative stability and reduced friction. By fine-tuning the proportions of PO, EPO, and EPME, it is

possible to develop bio-lubricant formulations that are both efficient and environmentally friendly, suitable for a wide range of diesel engine applications.

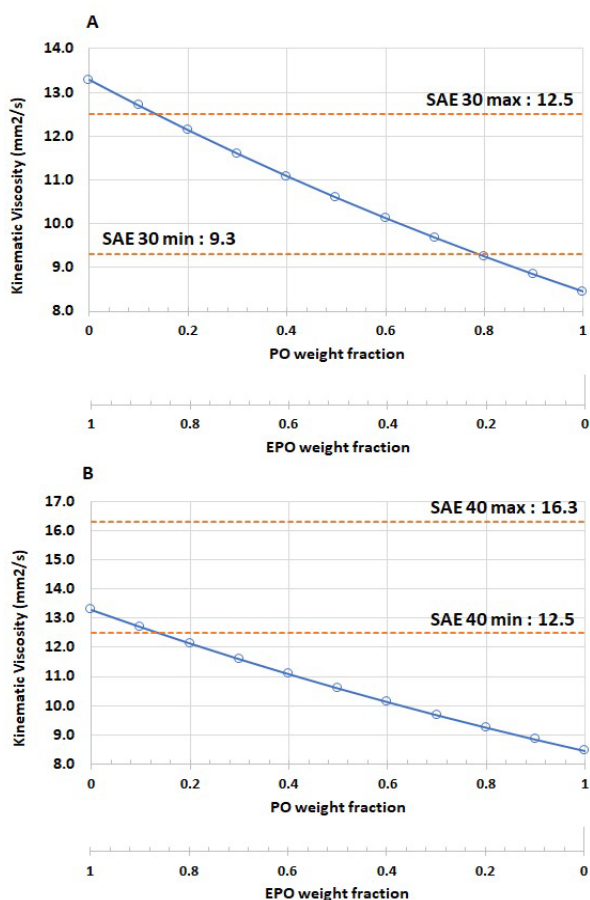


Fig. 2: The Viscosity map for mixtures of two base stocks (PO & EPO), SAE-30 (A) and SAE-40 (B)

5. Conclusion

- The study demonstrated that bio-lubricants derived from palm oil, such as palm olein and palm methyl ester, exhibited enhanced thermal-oxidative stability following chemical modifications. These changes raised the decomposition temperatures, allowing the bio-lubricants to better endure the high temperatures commonly encountered in diesel engines.
- Bio-lubricants were developed to meet the stringent viscosity requirements of SAE-30 and SAE-40 standards. This ensures that the bio-lubricants possess the appropriate flow characteristics to perform effectively in diesel engines, making them suitable for practical use in demanding conditions. Adhering to these standards is crucial for maintaining smooth and efficient engine operation.
- An important part of the study was using machine learning to predict and improve the properties of bio-lubricants. By using the BimolP tool, scientists calculated molecular descriptors to predict thermal-oxidative stability and lubricity. This method made the

formulation process more efficient and helped make quick decisions by predicting properties before doing expensive and time-consuming experiments.

- The chemical changes that improved thermal-oxidative stability also slightly increased the friction coefficient. This shows the challenge of balancing different properties in bio-lubricant formulations. Improving one property can affect another, so further optimization is needed to keep friction low while maintaining better thermal-oxidative stability. This highlights the ongoing effort to create bio-lubricants that perform well in multiple areas.

6. Recommendation

- Validation of the bio-lubricant formulation needs to be carried out with measurements to confirm predicted enhancements in thermal-oxidative stability and adherence to viscosity standards. These tests validated the reliability and effectiveness of the machine learning predictions and the overall formulation strategy.
- Further exploration of additional base stocks and their combinations could yield bio-lubricant formulations with even better performance characteristics. Investigating a wider range of palm oil derivatives and other renewable sources may lead to the discovery of new formulations with superior properties.
- Conducting long-term performance and endurance tests on diesel engines using these bio-lubricant formulations is essential. These tests will provide valuable insights into the durability and effectiveness of the bio-lubricants under real-world operating conditions, ensuring their reliability and efficiency over extended periods.

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Nomenclature

CoF	Coefficient of friction (–)
PO	Palm Olein
EPO	Epoxidized Palm Olein
POHMA	Palm Olein Hydroxy Methyl Amine
PME	Palm Methyl Ester
EPME	Epoxidized Palm Methyl Ester
PMEHMA	Palm Methyl Ester Hydroxy Methyl

Amine

Greek symbols

 η kinematic viscosity (mm²/s)

References

- 1) M.H. Jabal, A.R. Abdulmunem, H.S. Abd, "Experimental investigation of tribological characteristics and emissions with nonedible sunflower oil as a bio-lubricant," *Journal of The Air & Waste Management Association*, 69 (1) 109-118 (2019). Doi: 10.1080/10962247.2018.1523070
- 2) J.A. Cecilia, D.B. Plata, R.M.A. Saboya, F.M.T. de Luna, C.L. Cavalcante, and E. Rodríguez-Castellón, "An overview of the bio-lubricant production process: challenges and future perspectives," *Processes*, 8 (3) (2020). doi:10.3390/pr8030257.
- 3) F.J. Owuna, M.U. Dabai, M.A. Sokoto, S.M. Dangoggo, B.U. Bagudo, U.A. Birnin-Yauri, L.G. Hassan, I. Sada, A.L. Abubakar, and M.S. Jibrin, "Chemical modification of vegetable oils for the production of bio-lubricants using trimethylolpropane: a review," *Egyptian Journal of Petroleum*, 29 (1) 75–82 (2020). doi:10.1016/J.EJPE.2019.11.004.
- 4) M.A. Kalam, H.H. Masjuki, H.M. Cho, M.H. Mosarof, M.I. Mahmud, M.A. Chowdhury, and N.W.M. Zulkifli, "Influences of thermal-oxidative stability, and lubrication performance of biodegradable oil as an engine oil for improving the efficiency of heavy duty diesel engine," *Fuel*, 196 36–46 (2017). doi:10.1016/j.fuel.2017.01.071.
- 5) S. Arumugam, G. Sriram, and R. Ellappan, "Bio-lubricant-biodiesel combination of rapeseed oil: an experimental investigation on engine oil tribology, performance, and emissions of variable compression engine," *Energy*, 72 618–627 (2014). doi:10.1016/j.energy.2014.05.087.
- 6) A.R. Dey, and R.D. Misra, "Effect of infiltration of bio-lubricant on the performance of a compression ignition engine fuelled with biodiesel blends," *Clean Technol Environ Policy*, 19 (2) 553–563 (2017). doi:10.1007/s10098-016-1247-3.
- 7) B. Cahyono, A. Zuhdi, M. Fathallah, A. Youri, and A. Kahfi, "Durability of Diesel Engine Using Bio-lubricant and the Effect on Performance," 2021.
- 8) H.R. Amriya Tasneem, K.P. Ravikumar, and H. V. Ramakrishna, "Performance and wear debris characteristics of karanja biodiesel and bio-lubricant as a substitute in a compression ignition engine," *Fuel*, 319 (2022). doi:10.1016/j.fuel.2022.123870.
- 9) S.G. Muthurathinam & A.V. Perumal, "Synthesis, characterization and tribological investigation of vegetable methyl esters based bio-lubricants," *Industrial Crops and Products*, 203 1-10 (2023). doi: 10.1016/j.indcrop.2023.117098
- 10) P. Negi, Y. Singh, and K. Tiwari, "A review on the production and characterization methods of bio-based lubricants," in: *Mater Today Proc*, Elsevier Ltd, 2021: pp. 10503–10506. doi:10.1016/j.matpr.2020.12.1211.
- 11) K. Rama Rao Chebattina, V. Srinivas, G.V.S. Pranay, P. Vishwanath Krishna, and S.P. Jagadhi, "Tribological characteristics of Calophyllum ester based bio-lubricant - Commercial engine oil blends," in: *IOP Conf Ser Mater Sci Eng*, IOP Publishing Ltd, 2019. doi:10.1088/1757-899X/653/1/012013.
- 12) N.S. Ahmed, and A.M. Nassar, "Lubricating oil additives," *Tribology - Lubricants and Lubrication*, (2011). www.intechopen.com.
- 13) A.C. Opia, M.F. Bin Abdollah, M.K.A. Hamid, and I. Veza, "A review on bio-lubricants as an alternative green product: tribological performance, mechanism, challenges and future opportunities," *Tribology Online*, 18 (2) 18–33 (2023). doi:10.2474/trol.18.18.
- 14) N.M. Nor, D. Derawi, and J. Salimon, "Pengubahsuaian kimia minyak sawit terepoksida untuk aplikasi biopelincir," *Malaysian Journal of Analytical Sciences*, 21 (6) 1423–1431 (2017). doi:10.17576/mjas-2017-2106-25.
- 15) Z. Wan, Q. De Wang, D. Liu, and J. Liang, "Discovery of ester lubricants with low coefficient of friction on material surface via machine learning," *Chem Phys Lett*, 773 (2021). doi:10.1016/j.cplett.2021.138589.
- 16) X. Yu, and L. Huang, "Prediction of the onset temperature of decomposition of lubricant additives," *J Therm Anal Calorim*, 130 (2) 943–947 (2017). doi:10.1007/s10973-017-6511-1.
- 17) R.N. Sarma, and R. Vinu, "Current status and future prospects of bio-lubricants: properties and applications," *Lubricants*, 10 (4) (2022). doi:10.3390/lubricants10040070.
- 18) N. Mohd Nor, and J. Salimon, "Synthesis of Green-Renewable Bio-lubricant Base Stock from Malaysian Palm Oil," 2022.
- 19) L. Mairiza, Zuhra, M. Khadafi, Muhibbul, I. Budiman, and Y. Yunardi, "An overview of potential production of bio-lubricant in Indonesia," in: *IOP Conf Ser Earth Environ Sci*, IOP Publishing Ltd, 2022. doi:10.1088/1755-1315/951/1/012061.
- 20) N.A. Raof, H.A. Hamid, N.A. Mohamad Aziz, and R. Yunus, "Prospects of plant-based trimethylolpropane esters in the bio-lubricant formulation for various applications: a review," *Front Mech Eng*, 8 (2022). doi:10.3389/fmech.2022.833438.
- 21) E.J. de Sá Parente, L.B. de Oliveira, F.M.T. de Luna, and C.L. Cavalcante, "Integrated production of bio-lubricants and biodiesel: process simulation and technical-economic analysis," *Biomass Convers Biorefin*, (2023). doi:10.1007/s13399-023-04557-3.
- 22) S. Syahrullail, J.Y. Wira, A.H.M. Kameil, and W.N. Fawwaz, "Wear characteristic of RBD palm olein using four-ball tribotester," in: *AIP Conf Proc*, 2012: pp. 991–996. doi:10.1063/1.4704313.

- 23) M. Husnawan, H.H. Masjuki, and T.M.I. Mahlia, "The interest of combining two additives with palm olein as selected lubricant components," *Industrial Lubrication and Tribology*, **63** (3) 203–209 (2011). doi:10.1108/00368791111126626.
- 24) E.J. de Sá Parente, L.B. de Oliveira, F.M.T. de Luna, and C.L. Cavalcante, "Integrated production of bio-lubricants and biodiesel: process simulation and technical-economic analysis," *Biomass Convers Biorefin*, (2023). doi:10.1007/s13399-023-04557-3.
- 25) Z. Abd Maurad, H. Abu Hassan, and R. Ismail, "Process control for epoxidation of rbd palm olein," (2016).
- 26) I. Balde, C. Kane, A.K.D. Dime, S. Balde, and K. Ndiaye, "Vegetable oils epoxidation mechanisms," *World Journal of Analytical Chemistry*, **7** (1) 1–6 (2022). doi:10.12691/wjac-7-1-1.
- 27) R.A. Hartawan, M. Said, M. Faizal, J. Prianto, M. Juwita, and N. Aprianti, "Synthesis of epoxide as intermediate compounds for bio-lubricant production from crude palm oil," *Indonesian Journal of Fundamental and Applied Chemistry*, **7** (2) 42–50 (2022). doi:10.24845/ijfac.v7.i2.42.
- 28) M. Musik, E. Janus, R. Pelech, and Ł. Sałaciński, "Effective epoxidation of fatty acid methyl esters with hydrogen peroxide by the catalytic system h3pw12o40/ quaternary phosphonium salts," *Catalysts*, **11** (9) (2021). doi:10.3390/catal11091058.
- 29) M.H. Rahman, S. Shahriar, and P.L. Menezes, "Recent progress of machine learning algorithms for the oil and lubricant industry," *Lubricants*, **11** (7) (2023). doi:10.3390/lubricants11070289.
- 30) Y. Zhang, and X. Xu, "Machine learning decomposition onset temperature of lubricant additives," *J Mater Eng Perform*, **29** (10) 6605–6616 (2020). doi:10.1007/s11665-020-05146-5.
- 31) N. Salih, and J. Salimon, "A review on eco-friendly green bio-lubricants from renewable and sustainable plant oil sources," *Biointerface Res Appl Chem*, **11** (5) 13303–13327 (2021). doi:10.33263/BRIAC115.1330313327.
- 32) BRIN, "BimolP: Bio-lubricant Molecule Properties Analyzer," 000535521, 2023.
- 33) A. Pajankar, "Introduction to Python," in: Practical Python Data Visualization: A Fast Track Approach To Learning Data Visualization With Python, Apress, Berkeley, CA, 2021: pp. 1–16. doi:10.1007/978-1-4842-6455-3_1.
- 34) H. Moriwaki, Y.S. Tian, N. Kawashita, and T. Takagi, "Mordred: a molecular descriptor calculator," *J Cheminform*, **10** (1) (2018). doi:10.1186/s13321-018-0258-y.
- 35) SNI, "Klasifikasi dan spesifikasi – Pelumas – Bagian 5:Minyak lumas motor diesel putaran tinggi, SNI 7069-5:2021," 2021.
- 36) ASTM International, "Standard test method for kinematic viscosity of transparent and opaque liquids (and calculation of dynamic viscosity)." (astm d445-23)," (2023).
- 37) ASTM International, "Standard test method for calculating viscosity index from kinematic viscosity at 40 and 100 °c (astm d2270-16)," (2016).
- 38) D.J. Carlson, N.F. Giles, W.V. Wilding, and T.A. Knotts, "Improved liquid mixture viscosity predictions with the tlvme force field," *Fluid Phase Equilib*, **570** 113782 (2023). doi:10.1016/J.FLUID.2023.113782.
- 39) C.H. Chan, S.W. Tang, N.K. Mohd, W.H. Lim, S.K. Yeong, and Z. Idris, "Tribological behavior of bio-lubricant base stocks and additives," *Renewable and Sustainable Energy Reviews*, **93** 145–157 (2018). doi:10.1016/j.rser.2018.05.024.
- 40) C.K. Ho, K.B. McAuley, B.A. Peppley, "Biob lubricant through renewable hydrocarbons: A perspective for new opportunities," *Renewable and Sustainable Energy Reviews*, **113** 1-17 (2019), doi: 10.1016/j.rser.2019.109261
- 41) G.D. Giraldo, C.Z. Hernandez, J.F. Santa, R.B. Sierra, "Palm oil as a bio-lubricant: Literature review of processing parameters and tribological performance," *Journal of Industrial and Engineering Chemistry*, **107** 31–44 (2022), doi: 10.1016/j.jiec.2021.12.018.
- 42) U. Ahmad, S.R. Naqvi, I. Ali, M. Naqvi, S. Asif, A. Bokhari, D. Juchelkova, J.J. Klemes, "A review on properties, challenges and commercial aspects of eco-friendly bio-lubricants productions," *Chemosphere*, **309** 1-12 (2022), doi: 10.1016/j.chemosphere.2022.136622