Simulation of a bioavtur production process from non-edible vegetable oil

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Abstract. The increase in global aviation fuel demand has prompted ICAO to declare neutral carbon growth policy in 2050 by using bio based aviation fuel. The purpose of this study was to simulate the production of non-edible vegetable oil into bioavtur and obtain the most potential non-edible vegetable oil based on yield and conversion to be converted into bioavtur. Three potential sources to be converted into bioavtur are kosambi oil, nyamplung oil and kemiri sunan oil. This research was done by simulating of the hydroprocessing process with process simulator by varying the operating conditions on each raw material. Hydrotreating process was varied at 1-5 MPa pressure and temperature 250◦C-350◦C. The result showed the operating pressure with the highest conversion and yield are around 4MPa. While the operating temperature with high conversion and yield are above 290°C. Nyamplung oil has overall the largest yield and conversion than other non-edible vegetable oil with average 10% greater conversion and 3,3% greater yield at 2MPa.

1 Introduction

Commercialization of the aviation world has grown rapidly in the last 7 years, recorded in 2011 the number of domestic passenger flights of 59 million, this trend continues to grow until in 2015 the number of passengers increased to 75 million. Predicted this value will continue to grow in line with the equitable development of air transportation facilities in Indonesia. The increase in aviation also affects aviation fuel needs, by 2015 Indonesia needs 2.8 million kilo liters of avtur[1]. Bioavtur is widely used in conjunction with the campaign conducted by ICAO (International Commercial Airlines Association). Based on ICAO estimation, the aviation industry generates 2% of the total greenhouse gases in the atmosphere. In 2010, carbon dioxide accumulation in atmosphere reached 448 tons (Mt) which predicted to accumulate nearly 682 to 755 Mt by 2020, then 2700 Mt by 2050 if no action is taken. The increase in fuel demand and the potential increase in greenhouse gases prompted ICAO to declare neutral carbon growth by 2050 on aviation. In support of this policy the Indonesian government issues the Ministry of Energy and Mineral Resources's ministerial instruction number 12 of 2015 on bio-fuel mixing targets 5%. Moreover, bioenergy preferably works as supporting strategies for energy in Java and Bali [2].

Indonesia is one of the largest palm oil producing countries in the world. The Association of Indonesian Palm Oil Companies (GAPKI) noted that Indonesia's palm oil production in 2016 reached 34.5 million tons [3]. However, palm oil (edible-vegetable oil) usage as fuel, usually contradicted with the usage as food source and without proper planning it will cause negative impact [4]. Therefore, some non-edible vegetable oils found in tropical country potential to be converted into biofuels. This plant has excellent productivity with a large conversion such as; Nyamplung (22.2% free fatty acid content) [5], Kemiri Sunan (92.74% H-Fame conversion) [6] and Kosambi (C18 acid content: 57.8% wt) [7].

Last study bioavturs showed that bioavtur can be obtained from vegetable oils through the Hydrotreating process in laboratory, from which the Bioavures can be mixed up to a mixing ratio of 50% with conversion of up to 96% of macauba oil [8]. While, Gutierrez-Antonio et.al achieve 82% biofuel conversion from castor oil by simulating hydroprocessing process [9]. While this paper will simulate hydroprocessing by using kemiri sunan oil, kesambi oil and nyamplung oil.to produce biofuel.

It is hoped that this research can provide a yield and conversion prediction from non-edible vegetable oil into bioavtur..

2 Methodology

A process simulation was performed to evaluate the overall yield and product conversion. As previously described, this study used raw materials with 3 type of non-edible vegetables oil with a production capacity of 300 kg / hour. Then optimized at the hydrotreating stage by varying the operating conditions to obtain optimal operating conditions. The entire scheme of the process can be seen in Fig. 1[10]. In hydrotreating process based on those figure, process divided into three stages.

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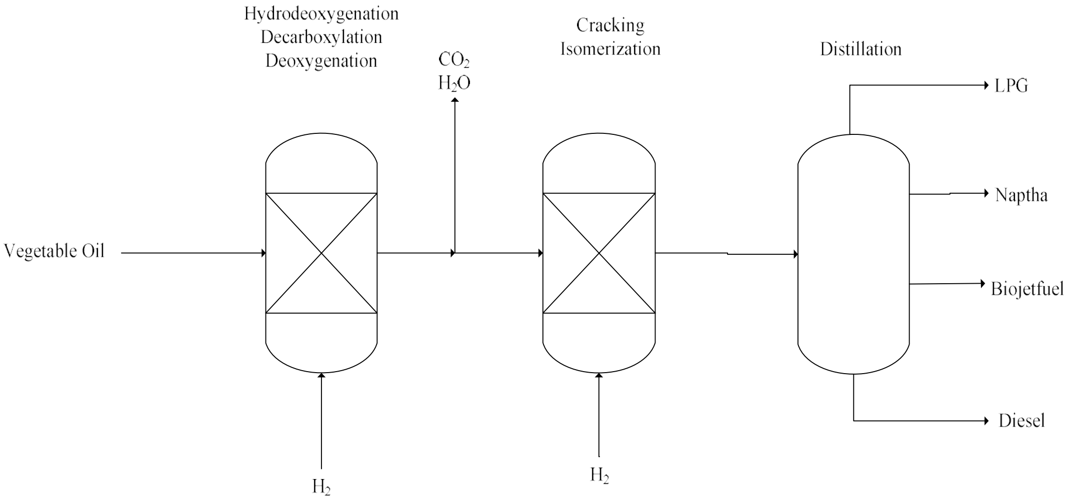


Fig. 1. Process Simulation Diagram [10]

First stage was hydrotreating to eliminate oxygen content in vegetable oil and produce long chain alkane. Second stage was hydrocracking which used to convert long alkane into shorter chain length. And the las stage was separation process, which used to divide product into bioLPG, biogasoline, bioavtur and renewable diesel.

2.1 Materials

The group of compounds undertaken in this study is divided into five, in the form of alkane compounds as the product, alkanol as intermediate, fatty acid as raw material, ester and additional compounds that are not sufficient to be grouped including water, hydrogen gas and carbon dioxide gas. Some of the compounds properties are not provided by simulation, so we use hypothetical compound to describe these compounds. All of the compound that we used are list based on reaction mechanism in hydrotreating mechanism in Kubickova[11]. Each of non-edible vegetable oil composistion in this simulation are listed in Table 1 based on their range of chain length and free fatty acid content. As seen in table 1, each of vegetable oil has different composition. Nyamplung oil has the largest FFA (free fatty acid) content, kemiri sunan has the largest C18 chain length content. Kesambi oil has the largest of C20 chain length. This composition difference will be evaluated due to yield and conversion that this vegetable oil reach.

Table 1. Non-Edible Vegetable Oil Composition

Fatty Acid	Nyamplung (%)[12]	Kemiri Sunan (%)[13]	Kosambi (%)[7]
C14	0.009	0	0.7
C16	14.26	10.1	8.7
C18	84.13	89.9	70.3
C20	1.66	0	20.2
C22	0.83	0	0
FFA	20	2.6	5.01

2.2 Hydrotreating

Hydroytreating process represents the formation of alkane carbon chains from fatty acids, by releasing oxygen groups in the form of carbon dioxide and water generally carried out in trickle bed reactors through the aid of CoMo /Al_2O_3 catalysts and hydrogen. This process was carried out at varying temperatures and pressures. Variations are performed at pressures of 1 MPa to 5 MPa and temperatures of 250°C to 350°C. The kinetic data incorporated in this process comprises kinetics including the decarboxylation and hydro-deoxigenation reactions taken from the results of laboratory experiments.

The hydrotreating process of vegetable oil is carried out using kinetics data provided from by Kubickova and Kubicka[11] which conduct comprehensive research on rapeseed oil. The reaction mechanism can be seen in [11], which provide two mechanism paths. This mechanism including hydrodeoxygenation which produce water as side product with larger hydrogen demand and hydrodecarboxylation which produce carbon dioxide as side product with lower hydrogen demand. The assumption that all of the chain lenght variety has same reactivity is used, to apply kinetics in kinetic reaction.

2.3 Hydrocracking

The hydrocracking/Izomerization is the process of reforming the alkane hydrocarbon chain into shorter or aromatic hydrocarbon alkane chains by reacting the alkane with hydrogen in a fixed bed reactor. This process can be found in the oil refinery industry to produce light hydrocarbons such as gasoline, aviation and diesel from heavy distillates and residues.[14] found that at a pressure of 50-60 bar and a temperature of 240◦C the maximum conversion to isomers was 32%, from 50% conversion to converted n-dodecane.

Gutierrez-Antonio et.al already use hydrocracking conversion data from steijns et.al to simulate biojet production by assuming normal alkanes with C15 to C18 atomic numbers having the same reactivity as n-dodecane showed realistic results [9].

This simulation used the same hydrocracking assumption as Gutierrez-Antonio et.al which assuming normal alkanes with C14 to C22 having same reactivity as n-dodeacane with equal product distribution. Therefore, hydrocracking formed in conversion reactor with 50% conversion.

2.4 Separation

From the scheme of the above process flow diagram, it is known that the output of this system has large variety of alkane chain including propane to C22, unreacted raw material, intermediates and side product. Separation is carried out on the remaining hydrogen gas, intermediates and unreacted vegetable oil into recycle stream. While carbon dioxide gas and water into purge stream. Main product, large variety of alkane chain are divided into four types of product based on chain length which are bioLPG (propane and butane), biogasoline (C5-C9), bioavtur (C10-C15) and renewable diesel (C16-C22). This separation process held by component splitter to reduce the complexity of system.

3 Result and Discussion

After simulating bioavtur production process for each vegetable oil and operating condition, we will validate the result. Analysis held by comparing yield and conversion trend for variety operating condition. The conversion and yield result also analyzed by comparing the composition of each vegetable oil.

Result of this simulation was validated by comparing properties of bioavtur produced from simulation and jet fuel standard. Simulated bioavture has 752 kg/m^3 density which still density range with Jet B Wide-Cut Kerosene with 750-801 kg/m^3 density at 15◦C. Specific comparation between product and standard be seen in table 2.

Table 2. Properties Comparation

Standard	AvturStd	Bioavtur
Lower Heating Value (MJ/kg)	42.8 (min)	44.46
Density (kg/m3) 15C	750-801	756.1
Boiling Point (C)	270 (max)	244
Viscosity @20C (cP)	n/a	1.837
Kinematic Viscosity @20C (cSt)	8.8 (max)	2.423

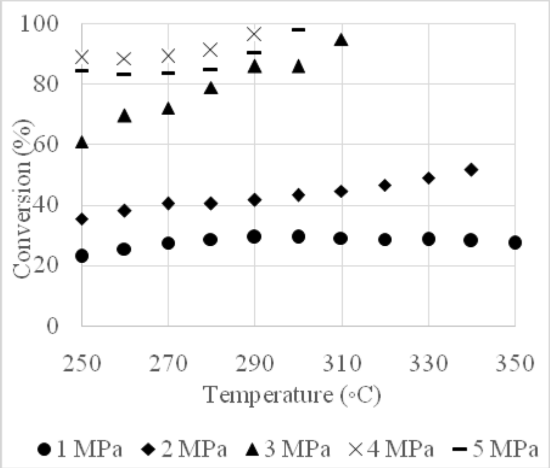
3.1 Yield and Conversion Result

Yield and Conversion of each vegetable oil was reviewed from the overall process of the system by varying the hydrotreating process conditions. Each conversion and yield result then presented in graphical at Fig.*2*, where the axial shows the temperature in C◦, the vertical axis showing yield and conversion in percent, and for each pressure variation has different mark in graph.

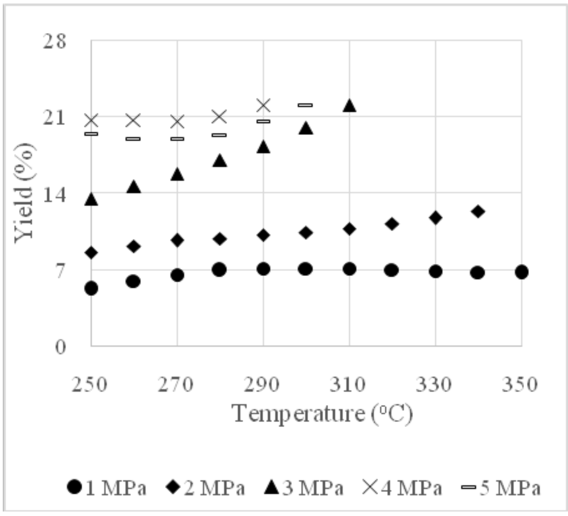
Each graph in Fig.2 shows the yield and conversion values for each temperature variation and the operating pressure applied to the kosambi, kemiri sunan and nyamplung oil. Based on the graph, yield and conversion values are directly proportional to operating temperatures with different slopes for each pressure, where the largest slope gained at 3MPa pressure. This trend also applied with pressure changes, increasing pressure cause increasing the value of yield and conversion from kemiri sunan, kosambi and nyamplung oil. The largest conversion increase only happened at 3MPa pressure comparing to other pressure.

However, at the temperature variation with the smallest pressure 1MPa, it shows a small increase in value of conversion from each vegetable oil from temperature range 250 ◦C to 290◦C, a temperature increase after 290 ◦C has no major effect for conversion values and it is tended to be constant with temperature increases in the range of 290 ◦C to 340 ◦C and decrease at 350 ◦C. At 2MPa pressure with temperature variation, yield and conversion consistently increase as temperature increases with small slopes. For all vegetable oil, yield and conversion big leap occurred at 3MPa pressure. Conversion increase nearly 20% at lowest temperature from pressure 2MPa to 3MPa. While, yield increase around 6% at lowest temperature from pressure 2MPa to 3MPa. This conversion increase occurs during temperature rise. Conversions above 90% for 3MPa pressure are achieved at 310 ◦C for most vegetable oil.

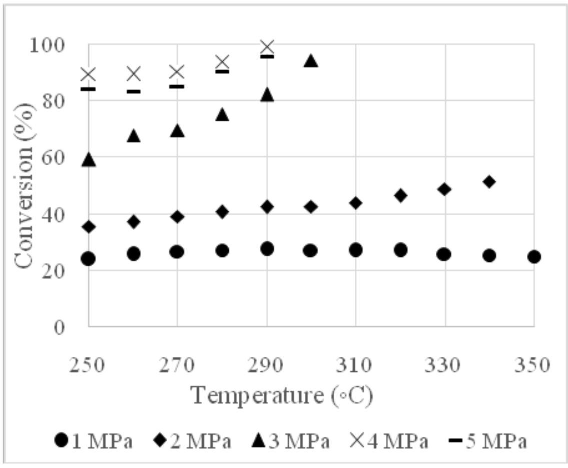
At 4MPa pressure, it tends to be more effective for lower temperatures (under 290◦C) because yield and conversion gap from lower pressure are much higher at that temperature range. While in the temperature range above 290◦C, although yield and conversion obtained is higher than 3MPa pressure but the increase is not significant. This conversion and yield trend happen for all the vegetable oil. At the 5MPa pressure evaluation, yield and conversion increments are not much different than the 4MPa pressure, although the conversion value is lower.



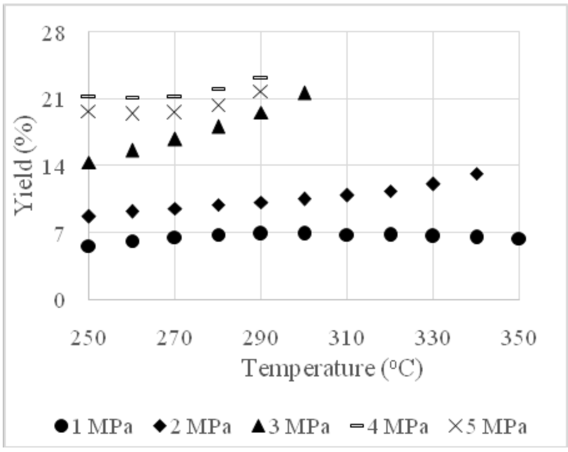
(a). Kosambi Oil Conversion



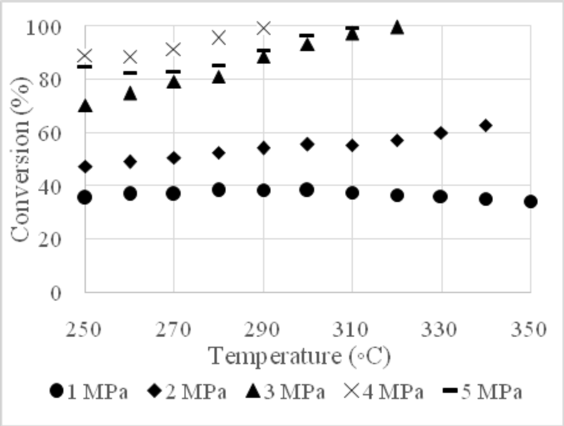
(b)Kosambi Oil Yield



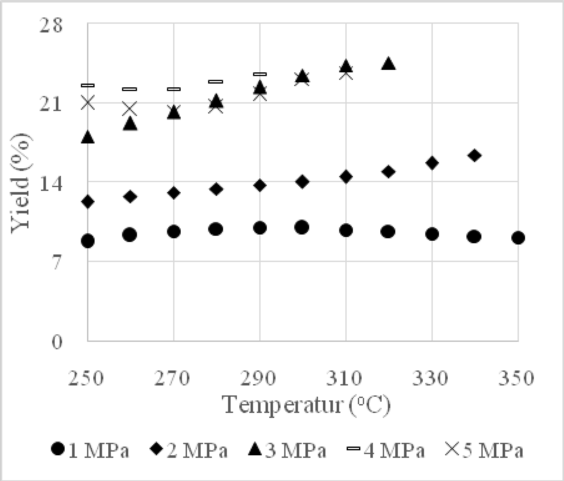
(c) Kemiri Sunan Oil Conversion



(d) Kemiri Sunan Oil Yield



(e)Nyamplung Oil Conversion



(f)Nyamplung Oil Yield

Fig.2. Variety of Yield and Conversion of Non-Edible Vegetable Oil

Overall for each vegetable oil, the conversion will tend to increase as the temperature rises at a pressure of 2 to 5MPa. While for 1MPa pressure the conversion tends to be consistent or decrease after temperature 290 ◦C. The most effective increase occurs at 3MPa pressure where the increase in conversion can rise up to 20%. Then at 4MPa pressure, the conversion is more effective at temperatures below 290 ◦C because the conversion gap is still greater than the 3MPa pressure. For all vegetable oils conversion is decreased when evaluated at 5 MPa pressure, although conversion difference is not too far compared to 4MPa pressure. Therefore, the operating pressure with the highest conversion and yield are around 4MPa. While the operating temperature with high conversion and yield are above 290 ◦C.

All this happening trend for yield and conversion for each vegetable oil are purely because of reaction kinetics and composition which will be discussed in the next sub-chapter.

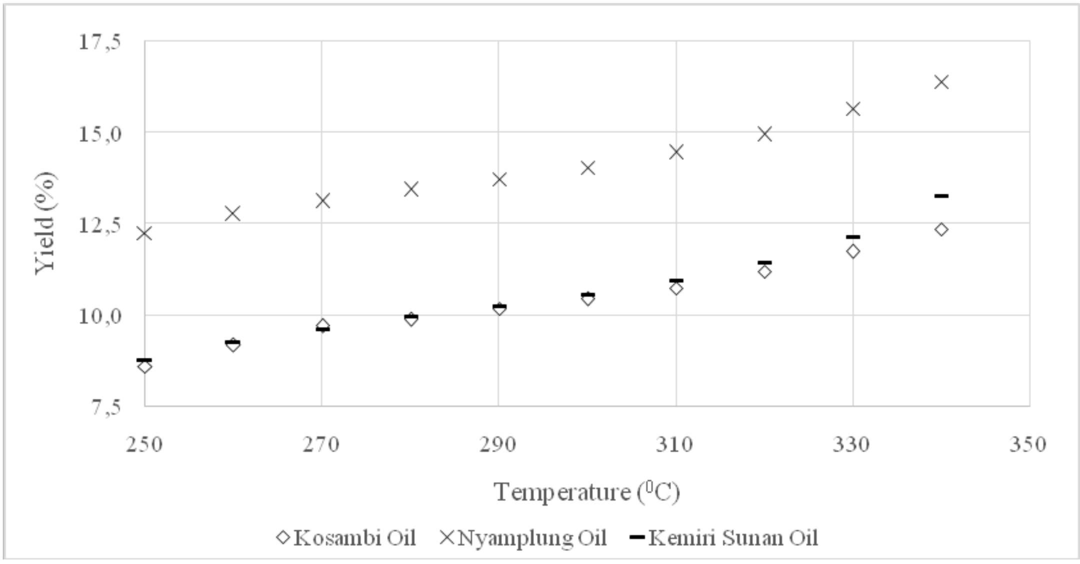
Based on the explanation above, the evaluation of the temperature is stopped at a certain higher temperature. Because at some point on those higher operating condition, mass balance from the system are negatives due to higher value of conversion (more than 100%) forced purge stream into negatives value. However, purge installation in system was done to anticipate the flow rate of recycle stream. A very big recycle stream will make the system not feasible. At higher temperatures the conversion becomes larger while the raw material inrush is kept constant. This will result in the system forcing the stream purge to be negative value makes the simulation result impossible. Therefore, variation of temperature at some point are not evaluate in this simulation.

3.2 Vegetable Oil Composition Effect

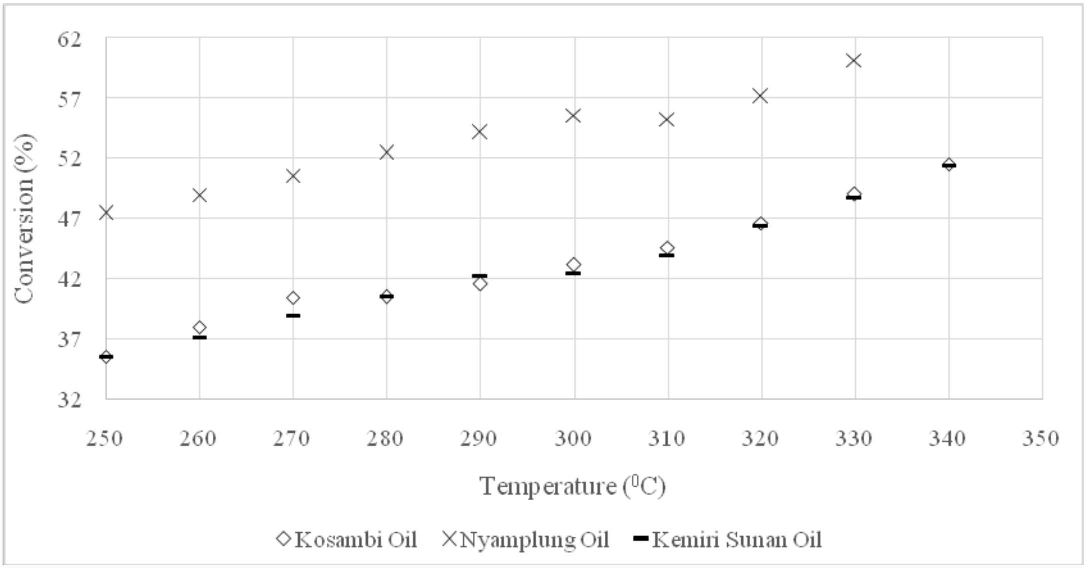
In this study, three types of vegetable oils are used; kesambi oil, kemiri sunan oil and nyaplung oil. Each composition of the vegetable oil is different so that the effect of the oil composition will be evaluated. Composition of each vegetable oil was showed in Table 1. The evaluation is performed on the oil composition of the conversion and yield. It is important to analyze vegetable oil composition effect. Because vegetable oil composition linked into reaction mechanism that simulate in this research.

The graph in Fig.3 (a) shows the bioavur yield of vegetable oil at a pressure of 2MPa with a temperature variation. 2MPa pressure is taken as a reference because at this pressure the complete yield data evaluated from various temperatures of 250 ◦C to 350 ◦C and the yield gradient in each vegetable oil are greater than at 1MPa. From the graph above seen as the rising temperatures tend to increase vegetable oil yields for all vegetable oils, this is supported by the increase of conversion from vegetable oil itself. The highest yield of was achieved from Nyamplung Oil with a value of 12,5% at the lowest temperature 250◦C followed by kemiri sunan and kesambi oil.

When viewed from the composition of vegetable oil, FFA content is quite influential on the value of the yield but limited only to affect the conversion. This showed by the largest conversion of nyamplung oil than other vegetable oil which has the largest FFA content around 20%, while other vegetable oil like kesambi and kemiri sunan only have 5.01% and 2.5% FFA.



(a) Vegetable oil yield at 2MPa with temperature variation



(b) Vegetable oil conversion at 2MPa with temperature variation

Fig.3. Variation of Vegetable Oil Yield and Conversion

To evaluate effect on bioavtur yields due to the composition of fatty acid chain length of each vegetable oil. we minimize the impact of conversion due to FFA, we will review vegetable oils with the lowest FFA levels which is kemiri sunan oil (2.6% FFA) and kesambi oil (5.01%). In Fig.3 (b) it showed that both of kosambi oil and kemiri sunan oil has the slightly the same number of conversion. However, if we evaluate Fig.3 (a) kemiri sunan tend to have better yield than kesambi oil. By comparing the fatty acid composition, kemiri sunan tend to have lower chain length of fatty acid while kesambi oil has longer fatty acid including 20% of arachidic acid (C20). As the temperature increase, yield gap between kemiri sunan and kosambi oil are larger with leap on kemiri sunan. This result showed that, vegetable oils that have shorter chain lengths will have greater bioavur yields more over with the increase of temperature.

4 Conclusion

In this study, bioavure production is simulated through hydroprocessing of non-edible vegetable oil with variation in Hydrotreating process to evaluated yield, conversion. The result showed Nyamplung oil has overall the largest yield and conversion due to largest FFA content. While, the operating pressure with the highest conversion and yield are around 4MPa. While the operating temperature with high conversion and yield are above 290 ◦C.

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References

1. Badan Pusat Statistik Indonesia Report, Statistik Transportasi Udara, BPS-Indonesia, Jakarta, (2016).
2. M. Gunter. International Journal of Technology. **9(**2). 257-266. (2018).
3. GAPKI Report, Gabungan Pengusaha Kelapa Sawit Indonesia, Jakarta, (2016)
4. M. M. Gui, K. T. Lee, S. Bhatia. Energy **133,** 1646-1653 (2008)
5. M. K. Charudatta, A. Ramanathan. Int J of Green Energy (2017)
6. E. Ramayeni, B. H. Susanto and D. F. Prakatama, IOP Conf. Ser.: Earth Environ. Sci. **105**, 012055 (2017)
7. C. Palanuvej, N. Vipunngun. J. Health Res.**4**,22 (2008)
8. V. P. Sousa, C. C. Cardoso, V. M. D. Pasa, Fuel Processing Technolgy**143**, 35-42 (2016)
9. C. Gutierrez-Antonio, G. Castro, D. L. Flores, S. A. Hernandes, Renewable and Sustainable Energy Reviews, 709-729 (2017).
10. L. Tao, W. Wang, Renewable and Sustainable Energy Reviews **53**, 801-822 (2016)
11. D. Kubickova, V. Tukac, Advances in Chemical Engineering **42**, 141-193 (2010).
12. M. Tjukup, S. Endang. Jurnal Natur Indonesia. **13,** 112-117 (2011)
13. D. F. Pratama, B. H. Susanto and E. Ramayeni, IOP Conf. Ser: Earth Environ. Sci. **105**, 012056 (2017).
14. M. Steijns, G. Froment, P. Jacobs, J. Utterhaeven, J. Weitkamp, Ind. Eng. Chem. Prod. Res. Dev. **20**. 654-660 (1981)