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Synthesis and Kinetic Model of Oleic Acid-based Epoxides by *In Situ* Peracid Mechanism

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Abstract

The global consumption of raw materials has shifted from the use of non-renewable materials to renewable materials. Studies on greener epoxidation by using vegetable oils to produce eco-friendly epoxides have also increased. In this study, the epoxidation of palm oleic acid was carried out by *in situ* generated performic acid. Fourier transform infrared spectroscopy of the products was conducted to confirm the success of the epoxidation. Lastly, a mathematical model was developed using the numerical integration of the 4th order Runge–Kutta method, and the results showed good agreement between the simulation and experimental data, which validates the kinetic model.

Keywords

Epoxidation, vegetables oil, palm oil

1 Introduction

Naturally, oil palm trees can produce several bunches containing hundreds of small oil palm fruit. Oil palm fruit is composed of the exocarp, mesocarp, endocarp, and kernel.[1] Oleic acid can be obtained from the oil palm fruits, which can be converted from a low-value product to a value-added product (epoxidised palm oleic acid, EPOA) through a chemical reaction called epoxidation. EPOA is also known as oxirane, containing cyclic ethers with a reactive three-membrane ring. The peroxyacid first needs to be generated *in situ* by reacting concentrated hydrogen peroxide with formic acid. *In situ* peracid was implemented in this study since this process is safer and produces a high epoxide yield. EPOA has been widely used as an intermediate product, such as stabilizer and plasticizer of polyvinylchloride, as well as a solvent to replace volatile organic solvents in paints.[2,3]

The cost-effectiveness and environmentally friendly material traits of vegetable oil renders vegetable oil a favourable alternative to produce epoxides as well as derivatives from epoxide.[4] To date, there are no studies on the effect of oxidising agent on the epoxidation process, while there are only a few studies pertaining to the degradation of epoxides, where the researchers attempt to control the process in order to achieve a high conversion of oxirane. The degradation process occurs after the maximum relative conversion to oxirane (RCO), which many researchers have not investigated. However, the degradation product can still be used as an alternative for synthesis with other chemical products such as coatings, adhesives, and paints. Owing to the lack of studies, degraded epoxides are not fully utilised in chemical synthesis and the chemical industry.[5] Thus, the objective of this study was to examine the effect of hydrogen peroxide concentration on the epoxidation of palm oleic acid. In addition, the effect of the addition of hydrogen peroxide, formic acid, and water on the degradation of epoxides was studied. Due to the high potential of EPOA for commercialisation, it is crucial to determine the reaction rates of the epoxidation and degradation processes, which will enable the chemical industry to scale up production. To fulfil this requirement, the reaction kinetics of the epoxidation and degradation processes was also studied for different concentrations of hydrogen peroxide.

2 Methodology

2.1 Materials

Oleic acid (concentration: 75 %) was purchased from Chung Chemical Sdn. Bhd., while formic acid (2 mol dm^{-3}, concentration: 85 %) and hydrogen peroxide (3.5 mol dm^{-3}, concentrations: 30, 35, and 40 %) were purchased from Merck Sdn. Bhd. For the titration process, hydrogen bromide (3.0 mol dm^{-3}, concentration: 48 %) was purchased from Qrec Sdn. Bhd., while crystal violet and glacial acetic acid (1 mol dm^{-3}, concentration: 100 %) were purchased from Merck Sdn. Bhd. In this study, molar ratios of formic acid : hydrogen peroxide : oleic acid were set at 1 : 1 : 1.

2.2 Experimental setup and procedure

The epoxidation reaction was carried out in a 500-ml beaker. A hot plate was used as the heater for the experiments. Firstly, 100 g of oleic acid was added into the 500-ml

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beaker equipped with a magnetic stirrer and thermometer, which were then immersed in a thermostatic water bath. The oleic acid was stirred at a constant speed of 300 rpm until the temperature reached 60 °C. The reaction was stirred continuously to prevent the explosion of hydrogen peroxide owing to the high concentration of this chemical reagent. The titration process was then initiated (and therefore, the experimental time began), where all of the chemicals were mixed every 5 min. Subsequently, 0.5 g of sample was taken from the beaker, added into a vial, and mixed with two droplets of crystal violet and 10 ml of glacial acetic acid. The mixed sample was titrated by subtracting the initial and final values of hydrogen bromide.

2.3 Analytical techniques

Experiments were conducted to determine the relative conversion to oxirane (*RCO*) by calculating the oxirane oxygen content (*OOC*) theoretically, and using a direct titration of hydrobromic (HBr) acid solution to indicate the degree of unsaturation in the palm oil in order to determine the *OOC* experimentally. The *RCO* (Eq. (1)) was determined based on the *OOC* value, which was determined theoretically (Eq. (2)) and experimentally (Eq. (3)).[6]

$$RCO = \frac{OOC_{\text{exp}}}{OOC_{\text{theor}}} \cdot 100 \quad (1)$$

$$OOC_{\text{theor}} = \left\{ \left(\frac{X_0}{A_{\text{i}}} \right) / \left[100 + \left(\frac{X_0}{2A_{\text{i}}} \right) \left(A_{\text{o}} \right) \right] \right\} \cdot A_{\text{o}} \cdot 100 \quad (2)$$

$$OOC_{\text{exp}} = 1.6 \cdot c \cdot \frac{(V - B)}{W} \quad (3)$$

X_0 is the initial iodine value, A_{i} is the molar mass of iodine, A_{o} is the molar mass of oxygen, c is molar concentration of HBr, B is the volume of the HBr solution used for the blank in millilitres (ml), V is the volume of HBr solution used for titration, and W is the weight of the sample. The experiment was repeated twice, and the samples were not purified at all.

2.4 Kinetic modelling

To develop the kinetic model of the epoxidation process, the main reactions involved in the epoxidation and degradation of the epoxidation process are as shown in Eqs. (4) and (5).

$$\text{FA} + \text{H}_2\text{O}_2 \underset{k_{12}}{\overset{k_{11}}{\rightleftarrows}} \text{PFA} + \text{H}_2\text{O} \quad (4)$$

$$\text{PFA} + \text{OA} \xrightarrow{k_{21}} \text{EPOA} + \text{FA} \quad (5)$$

FA, PFA and OA are formic acid, performic acid, and oleic acid, respectively, while k_{11}, k_{12}, and k_{21} are the kinetic constants. From the given epoxidation and degradation processes (Eqs. (4) and (5)), the differential equations for each species are derived in Eqs. (6)–(11).

$$\frac{\text{d}[\text{FA}]}{\text{d}t} = -k_{11}[\text{FA}][\text{H}_2\text{O}_2] + k_{12}[\text{PFA}][\text{H}_2\text{O}] + k_{21}[\text{PFA}][\text{OA}] \quad (6)$$

$$\frac{\text{d}[\text{H}_2\text{O}_2]}{\text{d}t} = -k_{11}[\text{FA}][\text{H}_2\text{O}_2] + k_{12}[\text{PFA}][\text{H}_2\text{O}] \quad (7)$$

$$\frac{\text{d}[\text{PFA}]}{\text{d}t} = k_{11}[\text{FA}][\text{H}_2\text{O}_2] - k_{12}[\text{PFA}][\text{H}_2\text{O}] - k_{21}[\text{PFA}][\text{OA}] \quad (8)$$

$$\frac{\text{d}[\text{H}_2\text{O}]}{\text{d}t} = k_{11}[\text{FA}][\text{H}_2\text{O}_2] - k_{12}[\text{PFA}][\text{H}_2\text{O}] \quad (9)$$

$$\frac{\text{d}[\text{OA}]}{\text{d}t} = -k_{21}[\text{PFA}][\text{OA}] \quad (10)$$

$$\frac{\text{d}[\text{EPOA}]}{\text{d}t} = k_{21}[\text{PFA}][\text{OA}] \quad (11)$$

The values were predicted using genetic algorithms in MATLAB software, where the algorithm can search for the ideal value of the process variable and fitting the experiment.[7] To prove the reliability of the parameter, the error, e, between the experiment and simulation needs to be minimised.

2.4 Fourier transform infrared (FTIR)

FTIR is an analytical technique used to identify organic, polymeric, and, in some cases, inorganic materials by using the FTIR spectrophotometer. In this case, FTIR was used to identify the oxirane ring group after alteration from carbon double bond. In this study, the functional groups of the samples were identified using a FTIR spectrometer (Spectrum One, Perkin Elmer, USA). The FTIR spectra were recorded within a wavenumber range of 400–4000 cm^{-1}, which is the mid-infrared region corresponding to the fundamental vibration modes of the molecules.[8,9]

3 Results and discussion

3.1 Effect of hydrogen peroxide on the epoxidation process

For the experiment, one manipulated variable was chosen (hydrogen peroxide concentration), whereas the reaction temperature, molar ratio, and stirring speed were selected as the controlled variables. Three hydrogen peroxide concentrations were selected, namely, 30, 35, and 50 %. The response variable was the *RCO* in percent (%), which is indicative of the epoxide yield. Three sets of experiments were performed, and the results are presented and discussed in this section. Hydrogen peroxide serves as an oxygen donor, which contributes active oxygen to the formic acid in order to form performic acid.[10]

The highest *RCO* was 62.18 %, which was achieved for a hydrogen peroxide concentration of 30 %, followed by those for a hydrogen peroxide concentration of 50 % and 35 %. The operating temperature, stirring speed, and molar ratio were fixed at 60 °C, 300 rpm, and 1 : 1 : 1, respectively. Fig. 1 shows that the *RCO* varied for different hydrogen peroxide concentrations, indicating that the hydrogen peroxide concentration had affected the epoxidation process. During the epoxidation process, the formic acid, which is a part of carboxylic acid, serves as an oxygen carrier, whereas the concentrated hydrogen peroxide serves as an oxygen donor. The *OOC* in the experiment was affected by the hydrogen peroxide concentration. To achieve a higher *OOC*, it was necessary to select a proper hydrogen peroxide concentration. Increasing the peroxy acid content in the reaction mixture increased the *OOC*.[11] This trend is similar to the results of other researchers, who found that a HP concentration of 35 % gives a fast reaction.[12,13] As the hydrogen peroxide concentration was increased in the reaction mixture, the peroxy acid concentration decreased.

Based on Fig. 1, the rate and stability of the reaction increased as the hydrogen peroxide concentration decreased. The *RCO* increased with the reaction time up to a certain value, as expected. It may be seen that the *RCO* was maximum at 15 min when the hydrogen peroxide concentration was 30 %. Interestingly, the *RCO* values were coincident for all hydrogen peroxide concentrations at 20 min. After the *RCO* reached its peak, it began to decrease with reaction time, and had the experiment proceeded for several hours, the *RCO* would have eventually reached 0 %. Based on the result, it can be concluded that different vegetable oil produces different conversion to oxirane based on hydrogen peroxide concentration. Therefore, hydrogen peroxide was used as a strong oxidant agent.

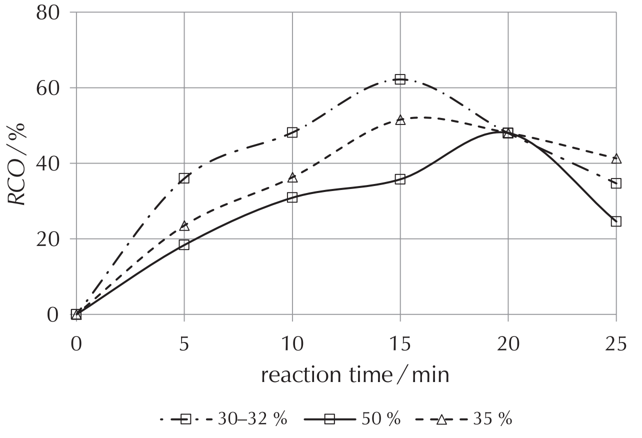

Fig. 1 – Effect of hydrogen peroxide concentration on the RCO

The functional groups contained in the sample can be determined using FTIR spectroscopy. The FTIR spectrometer measures the absorption of infrared radiation by the sample with respect to the wavenumber. The disappearance of the olefin functional group at 3010 cm^{-1} indicated the conversion of a double bond into an epoxy group, as shown in Fig. 2. This can be proven by the existence of the peak at 721 cm^{-1}, indicating the presence of an epoxide group. The peaks at 1710 and 1180 cm^{-1} revealed the presence of the C=O and C−O−C functional groups. The terminal methyl group of the triglyceride chains showed a strong band of C−H stretching at 2920 cm^{-1}, while the saturated fatty acid of methylene moieties showed a band of CH$_2$ stretching at 2850 cm^{-1}. The pre-development of a peak at 3410 cm^{-1} indicated the presence of hydroxyl group, suggesting the success of oxirane ring opening. High hydrogen peroxide concentration can be harmful to human skin, and therefore, this concentration is too acidic and hazardous for cosmetic purposes (when using 50 %).[14] This finding was similar to the previous work of several researchers.[15,16]

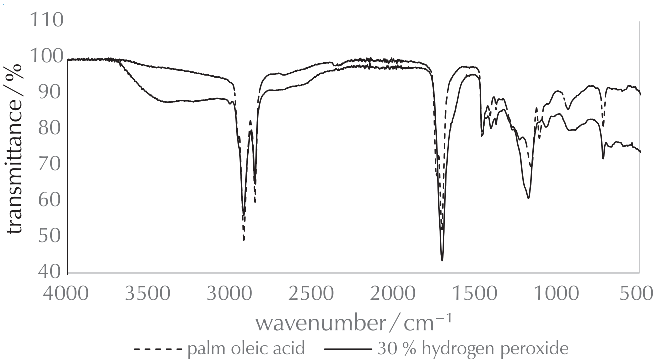

Fig. 2 – Comparison of FTIR spectra of palm oleic acid and EPOA with a hydrogen peroxide concentration of 30 %

The functional groups were similar for all samples, but the intensities of the FTIR spectra were different. In general, the intensity of the FTIR spectra varied, depending on the hydrogen peroxide concentration. Fig. 3 shows the peak intensities for the O−H, C=O, C−O−C, and C−H functional groups. In general, there was a significant difference in the peak size, where the peaks were sharper for the sample with hydrogen peroxide concentration of 30 % compared with those for other samples. There were slight differences in the wavenumber of the peaks for the C=O, O−H and C−H stretching, and the intensity was more pronounced for the sample with a hydrogen peroxide concentration of 35 %. The intensities of all functional groups for all samples are summarised in Table 1.

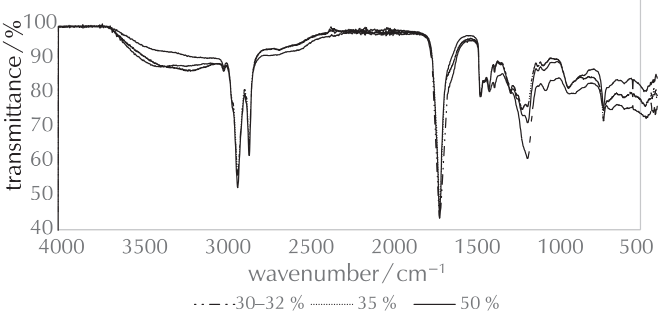

Fig. 3 – FTIR spectra for all EPOA samples

Table 1 – Intensities of FTIR spectra for all samples

Functional group	Intensity (*y*-axis)		
	30 %*	35 %*	50 %*
C=O stretching	4.35	4.61	5.23
C−O−C stretching	6.09	7.13	7.54
C−H stretching (CH_2)	6.48	6.50	6.16
C−H stretching (CH_3)	5.60	5.63	5.23
C−O−C asymmetric bending	7.18	7.18	7.13

* Hydrogen peroxide concentration

A pycnometer was used to determine the difference in density of all samples. The pycnometer determines the density of a liquid sample by removing air from the sample, followed by introducing a portion of liquid under vacuum. The densities of the EPOA samples are tabulated in Table 2. The sample with a hydrogen peroxide concentration of 35 % had the highest density (0.8830 g cm^{-3}), whereas the sample with a hydrogen peroxide concentration of 50 % had the lowest density (0.8456 g cm^{-3}). The densities were similar for the samples with a hydrogen peroxide concentration of 30 % and 35 %, indicating that the densities were quite similar even though the method of sample preparation was slightly different. In general, the densities of all samples were similar and within range.

Table 2 – Densities for all samples

EPOA sample	Density / g cm^{-3}
hydrogen peroxide concentration: 30 %	0.8806
hydrogen peroxide concentration: 35 %	0.8830
hydrogen peroxide concentration: 50 %	0.8456

3.2 Kinetic data of the epoxidation process for the EPOA samples with different hydrogen peroxide concentrations

Kinetic modelling was performed using MATLAB software to determine the optimal reaction conditions for the epoxidation process and the reaction rate values, *k*, as summarised in Table 3. The reaction rates, *k*, of the experimental data correspond to the initial concentration (1.4714 mol l^{-1}) for all chemicals (H_2O_2, FA, and OA). Activation energy can be hailed as the most important property in any kinetically controlled chemical reaction.[17,18] Here, *k* denotes a specific reaction rate; the higher the value, the faster the reaction. The hydrogen peroxide concentration is the main factor affecting the reaction rate for all samples. The minimising function available in *MATLAB* was used in order to determine the best curve fit and estimate the rate constants.[19] A comparison between simulation and experimental data based on kinetic reaction shown in Table 3 is plotted in Figs 4–6. It can also be observed that the hydrogen peroxide was totally consumed, as indicated hydrogen peroxide towards the end of the reaction.[20] The typical trend was that the oxirane content firstly increased at a reaction time of 0–15 min, followed by a decrease thereafter. In general, there was a good fit between the experimental and simulation values.

Table 3 – Simulation data. The initial concentrations of H_2O_2, FA, and OA were 1.4714 mol l^{-1}.

Hydrogen peroxide concentration / %	k_{11}	k_{12}	k_{21}	Mean error
30	0.3649	15.000	1.5828	0.2243
35	0.4156	12.599	0.7716	0.1201
50	0.1834	15.000	0.9288	0.1823

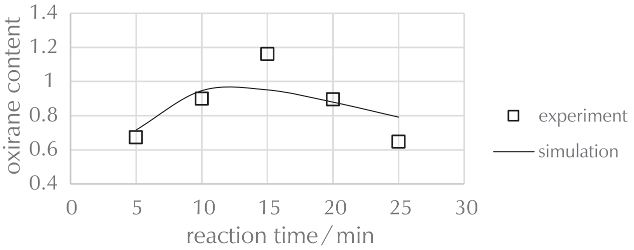

Fig. 4 – Comparison of the oxirane content between experiment and simulation for the EPOA sample with a hydrogen peroxide concentration of 30 %

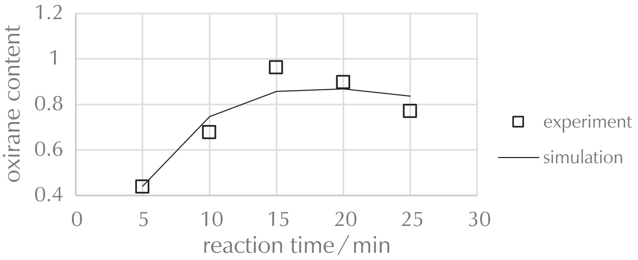

Fig. 5 – Comparison of the oxirane content between experiment and simulation for the EPOA sample with a hydrogen peroxide concentration of 35 %

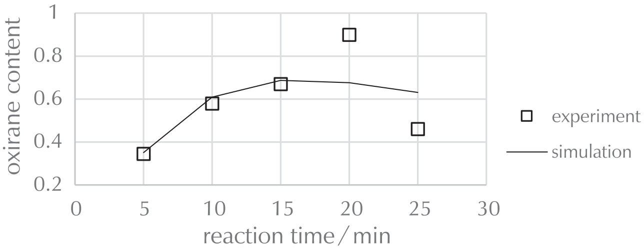

Fig. 6 – Comparison of the oxirane content between experiment and simulation for the EPOA sample with a hydrogen peroxide concentration of 50 %

4 Conclusion

In this study, palm oleic acid was used to produce epoxidised palm oleic acid. Performic acid (HCOOOH) was generated *in situ* during the epoxidation process. In the first phase, this study was focused on determining the optimal hydrogen peroxide concentration that would maximise the *RCO*. Three hydrogen peroxide concentrations were considered: 30 %, 35 %, and 50 %. Three sets of experiments were run to determine the *RCO* and the optimal hydrogen peroxide concentration at a constant temperature of 60 °C, stirring speed of 300 rpm, and reaction time of 35 min. In addition, a kinetic model was developed for both the epoxidation and degradation processes, by developing the kinetic model of palm kernel oil, using the differential method and applying the Runge–Kutta method. Overall, a high epoxide yield was obtained, and with the kinetic parameters, the production of epoxide can be scaled up for large-scale production.

References
Literatura

1. *P. K. Gamage, M. O. Brien, L. Karunanayake*, Epoxidation of Some Vegetable Oils and Their Hydrolysed Products With Peroxyformic Acid – Optimised to Industrial Scale, J. Natl. Sci. **37** (2009) 229–240, doi: https://doi.org/10.4038/jnsfsr.v37i4.1469.
2. *M. J. Jalil1, M. S. M. Zaini, A. F. M. Yamin, I. S. Azmi, S. H. Chang, N. Morad, A. Hadi*, Synthesis and Physicochemical Properties Of Epoxidized Oleic Acid-Based Palm Oil, IOP Conf. Ser. Earth Environ. Sci. **291** (1) (2019) 012046, doi: https://doi.org/10.1088/1755-1315/291/1/012046.
3. *P. Minyak, S. Olein, T. Sebagai, B. Keterbaharuan, A. Peroksi*, Preparation of Epoxidized Palm Olein as Renewable Material by Using Peroxy Acids, Malay. J. Anal. Sci. **18** (3) (2014) 584–591, url: http://www.ukm.my/mjas/v18_n3/Darfizzi_18_3_12.pdf.
4. *M. J. Jalil, A. Hadi, N. Mora, S. H. Chang, A. F. M. Yamin, M. S. M. Zaini*, Kinetics of Epoxidized Oleic Acid Derived From Palm Oil by *In Situ* Generated Performic Acid, Kem. Ind. **68** (5-6) (2019) 181–187, doi: https://doi.org/10.15255/KUI.2018.039.
5. *A. E. Kale, D. G. Goswami, P. S. Zade, M. B. Mandake,* Recent Advances in Epoxidation of Vegetable Oils, J. Emerging Tech. Innovative Res. **4** (4) (2017) 171–175, url: https://www.jetir.org/papers/JETIR1704042.pdf.
6. *S. Silviana, D. D. Anggoro, A. C. Kumoro,* Kinetics Study of Waste Cooking Oil Epoxidation with Peroxyacetic Acid Using Acid Catalysts, Rasayan J. Chem. **12** (3) (2019) 1369–1374, doi: https://doi.org/10.31788/RJC.2019.1235190.
7. *A. B. Kousaalya, S.D. Beyene, V. Gopal, B. Ayalew, S. Pilla,* Green Epoxy Synthesized From Perilla Frutescens: A Study on Epoxidation and Oxirane Cleavage Kinetics of High-Linolenic Oil, Ind. Crops Prod. **123** (1) (2018) 25–34, doi: https://doi.org/10.1016/j.indcrop.2018.06.047.
8. *M. J. Jalil, M. S. M. Zaini, A. F. M. Yamin, N. Morad, A. Hadi*, Degradation of Catalytic Epoxidation of Oleic Acid Palm Oil by *In Situ* Performic Acid, J. Phys. Conf. Ser. **1349** (2019) 012001, doi: https://doi.org/10.1088/1742-6596/1349/1/012001.
9. *M. J. Jalil, S. Khatijah Jamaludin, A. Rafizan, M. Daud*, Degradation Oxirane Ring Kinetics of Epoxidized Palm Kernel Oil-Based Crude Oleic Acid, Chem. Chem. Technol. **12** (3) (2018) 296–299, doi: https://doi.org/10.23939/chcht12.03.296.
10. *X. Cai, J. L. Zheng, A. F. Aguilera, L. Vernières-Hassimi, P. Tolvanen, T. Salmi, S. Leveneur*, Influence of Ring-Opening Reactions on the Kinetics of Cottonseed Oil Epoxidation, Int. J. Chem. Kinet. **50** (10) (2018) 1–16, doi: https://doi.org/10.1002/Kin.21208.
11. *E. Vanags, M. Kirpluks, U. Cabulis, Z. Walterova*, Highly Functional Polyol Synthesis from Epoxidized Tall Oil Fatty Acids, J. Renew. Mater. **6** (7) (2018) 764–771, doi: https://doi.org/10.7569/Jrm.2018.634111.
12. *M. J. Jalil, A. F. M. Yamin, M. S M. Zaini, N. Murad, A. Hadi*, Synthesis of Epoxidized Oleic Acid-Based Palm Oil by Peracid Mechanism, IOP Conf. Ser.: Mater. Sci. Eng. **551** (3) (2019) 012120, doi: https://doi.org/10.1088/1757-899X/551/1/012120.
13. *M. J. Jalil, A. F. M. Yamin, S. H. Chang, I. S. Azmi, N. Morad*, Selective Epoxidation of Crude Oleic Acid-Palm Oil with *In Situ* Generated Performic Acid, Int. J. Eng. Technol. **7** (4) (2018) 152–155, url: https://www.sciencepubco.com/index.php/ijet/article/view/24423.
14. *R. Turco, R. Tesser, R. Vitiello, Russo, V. S. Andini, M. Di Serio,* Synthesis of Biolubricant Basestocks From Epoxidized Soybean Oil, Catalysts **7** (10) (2017) 309, doi: https://doi.org/10.3390/catal7100309.
15. *F. Ezzah, A. Latif, Z. Z. Abidin, F. Cordona, D. R. A. Biak, P. M. D. Tahir, K. Abdan, K. E. Liew,* Physicochemical, Structural and Mechanical Evaluation of Bio-based Epoxidized Jatropha Oil Blended with Amine-Cured Epoxy Resin as New Hybrid Matrix, J. Eng. Sci. Technol. **14** (2) (2019) 1071–1087, url: https://jestec.taylors.edu.my/Vol%2014%20issue%202%20April%202019/14_2_38.pdf.
16. *N. M. Nor, D. Derawi, J. Salimon,* Chemical Modification of Epoxidized Palm Oil for Biolubricant Application, Malays. J. Anal. Sci. **12** (6) (2017) 1423–1431, doi: https://doi.org/10.17576/mjas-2017-2106-25.
17. *A. A. Beltrán Osuna, L. A. Boyacá Mendivelso*, Two-Phase Kinetic Model for Epoxidation of Soybean Oil, Ing. Investig. **30** (2) (2010) 188–196, url: http://www.scielo.org.co/scielo.php?pid=S0120-56092010000200019&script=sci_arttext&tlng=en.
18. *X. Cai, J. L. Zheng, A. F. Aguilere, L. V. Hassimi, P. Tolvanen, T. Salmi, S. Leveneur,* Influence of Ring-Opening Reactions on the Kinetics of Cottonseed Oil Epoxidation, Int. J. Chem. Kinet. **50** (10) (2018) 726–741, doi: https://doi.org/10.1002/kin.21208.
19. *A. F. M. Yamin, M. J. Jalil, I. Adnan, V. G. Vsiduru*, Numerical Modeling of Epoxidation Palm Kernel Oil Based Oleic Acid, Int. J. Eng. Technol. **7** (4) (2018) 123–126, doi: https://doi.org/10.14419/Ijet.V7i4.40.24417.
20. *L. Ifa, T. Syarif, Z. Sabara, N. Nurjannah, M. Munira, F. Aryani*, Study on The Kinetics of Epoxidation Reaction of RBD Palm Olein, IOP Conf. Ser. Earth Environ. Sci. **175** (1) (2018) 012035, doi: https://doi.org/10.1088/1755-1315/175/1/012035.

SAŽETAK

Sinteza epoksida i kinetički model epoksidacije oleinske kiseline *in situ* mehanizmom permravlje kiseline

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Upotreba sirovina na svjetskoj razini prešla je s neobnovljivih na obnovljive materijale. Također, intenzivirala su se istraživanja vezana uz zeleniju epoksidaciju primjenom biljnih ulja u proizvodnji ekološki prihvatljivih epoksida. U ovoj studiji, provedena je epoksidacija oleinske kiseline iz palmi primjenom *in situ* nastale permravlje kiseline. FTIR analiza produkata primijenjena je za potvrdu uspješnosti procesa epoksidacije. Naposljetku, primjenom metode Runge–Kutta 4. reda, razvijen je matematički model. Dobro slaganje simuliranih i eksperimentalnih podataka potvrdilo je ispravnost razvijenog kinetičkog modela.

Ključne riječi
Epoksidacija, biljna ulja, palmino ulje

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