https://doi.org/10.15255/KUI.2020.016
KUI-3/2021
Original scientific paper
Received March 30, 2020
Accepted July 27, 2020

High Yield Dihydroxystearic Acid (DHSA) Based on Kinetic Model from Epoxidized Palm Oil

M. J. Jalil,[a*] *K. A. Kamal*,[a] *A. F. B. M. Yamin*,[a] *I. S. Azmi*,[b] *M. H. Hassan*,[a] *A. R. Hidayu*,[b] and *K. N. Ismail*[c]

[a] Faculty of Chemical Engineering, Universiti Teknologi MARA Cawangan Pulau Pinang, Kampus Permatang Puah, 13 500 Permatang Pauh, Pulau Pinang
[b] Faculty of Chemical Engineering, Universiti Teknologi Mara Cawangan Johor Kampus Pasir Gudang, 81 750 Masai, Johor
[c] Faculty of Chemical Engineering, Universiti Teknologi MARA, 40 450 Shah Alam, Selangor

Abstract

In recent years, studies related to the epoxidation of fatty acids have garnered much interest due to the rising demand for eco-friendly epoxides derived from vegetable oils. From the epoxidation reaction, there is a side reaction involving epoxide and water. This reaction produces a by-product – dihydroxystearic acid ($C_{18}H_{36}O_4$, DHSA). DHSA is one of the chemical precursors in the production of cosmetic products. Therefore, a kinetic model was developed to determine the optimised epoxidation process and concentration of DHSA, where each of the reactions was identified. The kinetic rate, *k* parameters obtained were: k_{11} = 6.6442, k_{12} = 11.0185, k_{21} = 0.1026 for epoxidation palm oleic acid, and k_{41} = 0.0021, k_{51} = 0.0142 in degradation process. The minimum error of the simulation was 0.0937. In addition, DHSA yield optimisation was done through Taguchi method, and the optimum conditions obtained were H_2O_2/oleic acid – OA unsaturation molar ratio 1 : 1 (level 2), formic acid – FA/OA unsaturation molar ratio 0.5 : 1 (level 1), temperature 35 °C (level 1), and agitation speed 100 rpm (level 1). A high yield of DHSA can be achieved under these conditions.

Keywords

Epoxidation, kinetic rate, MATLAB, DHSA, Taguchi

1 Introduction

The growth in vegetable oil demand has increased compared to the petroleum-based polymer.[1] Since petroleum causes environmental pollution concerns, vegetable oil has become an alternative in the production of the epoxide. In the epoxidation reaction of vegetable oil, oxirane ring-opening, known as epoxide ring degradation, will occur.[2] The oxirane ring-opening depletes the yield and can cause high peroxide values of epoxidized vegetable oils, so the opening needs to be minimised.[3] The commercial production of palm oil is quite high compared to that of other vegetable oils.[4] The low cost of palm oil makes studies on the synthesis and oxirane cleavage of palm oil more practical and economical.[5] Epoxidized palm oil (EPO) can be obtained by reacting to the double bond of oil with peroxy acid that is generated *in situ* by reacting with concentrated hydrogen peroxide (H_2O_2) and formic acid (CH_2O_2, FA) in the presence of mineral salt as a catalyst.[2] The EPO can be used as a raw material in the manufacture of a wide range of products, such as paint, plastic, and adhesives. Besides, EPO is obtained from renewable resources, and can be regarded as biodegradable and non-toxic. Hence, it is suitable in replacing petroleum, since petroleum is toxic and harmful to the environment.

In this study, the oxirane-ring degradation of epoxidation palm oil was determined through *MATLAB* simulation. *Ode45* is one of the tools in *MATLAB* designed to work with differential equations. The benefit of this tool is its ability to determine the reaction rate of the epoxidation and degradation of EPO. Nevertheless, the epoxy that reacts with water produces DHSA. The physical appearance of DHSA is white and tasteless with an acid odour, and is non-irritating to the skin.[6] It is suitable for cosmetic ingredients. As the cosmetic industry is gradually increasing, it is suitable to produce a large amount of DHSA.[7] However, literature on the optimisation of DHSA production is still lacking and has only a few references. Thus, in this paper, the optimisation of DHSA production will be studied by the Taguchi method, and by referring the data from the simulation.

2 Methodology

2.1 Kinetic model

Two main reactions involved in epoxidation of palm oil can be illustrated in Eqs. 1 and 2, while, the degradation of epoxidation is described in Eqs. 3, 4, and 5.

$$\mathrm{FA} + \mathrm{H_2O_2} \underset{k12}{\overset{k11}{\rightleftarrows}} \mathrm{PFA} + \mathrm{H_2O} \quad (1)$$

$$\mathrm{PFA} + \mathrm{OA} \xrightarrow{k21} \mathrm{EPOXY} + \mathrm{FA} \quad (2)$$

$$\mathrm{EPOXY} + \mathrm{H_2O} \xrightarrow{k31} \mathrm{DHSA} \quad (3)$$

$$\mathrm{EPOXY} + \mathrm{H_2O_2} \xrightarrow{k41} \mathrm{DEG1} \quad (4)$$

$$\mathrm{EPOXY} + \mathrm{FA} \xrightarrow{k51} \mathrm{DEG2} \quad (5)$$

* Corresponding author: Mohd Jumain Jalil
Email: mjumain0686@uitm.edu.my

where FA, H_2O_2, PFA, H_2O, OA, EPOXY, and DHSA are formic acid, hydrogen peroxide, performic acid, water, oleic acid, epoxide vegetable oil, and dihydroxystearic acid, respectively. From the given epoxidation and degradation process, the differential equations that describe each species are further derived as follows:

$$\frac{d[\mathrm{FA}]}{\mathrm{d}t} = -k_{11}[\mathrm{FA}][\mathrm{H_2O_2}] + k_{12}[\mathrm{PFA}][\mathrm{H_2O}] + k_{21}[\mathrm{PFA}][\mathrm{OA}] - k_{22}[\mathrm{EPOXY}][\mathrm{FA}] - k_{51}[\mathrm{EPOXY}][\mathrm{FA}] + k_{52}[\mathrm{DEG2}] \quad (6)$$

$$\frac{d[\mathrm{H_2O_2}]}{\mathrm{d}t} = -k_{11}[\mathrm{FA}][\mathrm{H_2O_2}] + k_{12}[\mathrm{PFA}][\mathrm{H_2O}] - k_{41}[\mathrm{EPOXY}][\mathrm{H_2O_2}] + k_{42}[\mathrm{DEG2}] \quad (7)$$

$$\frac{d[\mathrm{PFA}]}{\mathrm{d}t} = k_{11}[\mathrm{FA}][\mathrm{H_2O_2}] - k_{12}[\mathrm{PFA}][\mathrm{H_2O}] - k_{21}[\mathrm{PFA}][\mathrm{OA}] + k_{22}[\mathrm{EPOXY}][\mathrm{FA}] \quad (8)$$

$$\frac{d[\mathrm{H_2O}]}{\mathrm{d}t} = k_{11}[\mathrm{FA}][\mathrm{H_2O_2}] - k_{12}[\mathrm{PFA}][\mathrm{H_2O}] - k_{31}[\mathrm{H_2O}][\mathrm{EPOXY}] + k_{32}[\mathrm{DHSA}] \quad (9)$$

$$\frac{d[\mathrm{OA}]}{\mathrm{d}t} = -k_{21}[\mathrm{PFA}][\mathrm{OA}] + k_{22}[\mathrm{EPOXY}][\mathrm{FA}] \quad (10)$$

$$\frac{d[\mathrm{EPOXY}]}{\mathrm{d}t} = k_{21}[\mathrm{PFA}][\mathrm{OA}] - k_{22}[\mathrm{EPOXY}][\mathrm{FA}] - k_{31}[\mathrm{EPOXY}][\mathrm{H_2O}] + k_{32}[\mathrm{EPOXY}][\mathrm{H_2O}] \quad (11)$$

$$\frac{d[\mathrm{DHSA}]}{\mathrm{d}t} = k_{31}[\mathrm{EPOXY}][\mathrm{H_2O}] - k_{32}[\mathrm{DHSA}] \quad (12)$$

$$\frac{d[\mathrm{DEG1}]}{\mathrm{d}t} = k_{41}[\mathrm{EPOXY}][\mathrm{H_2O_2}] - k_{42}[\mathrm{DEG1}] \quad (13)$$

$$\frac{d[\mathrm{DEG2}]}{\mathrm{d}t} = k_{51}[\mathrm{EPOXY}][\mathrm{FA}] - k_{52}[\mathrm{DEG2}] \quad (14)$$

To determine the rate coefficient numerically, parametric studies were conducted. There were two computing processes involved, which solved a set of differential equations (Eqs. 6–14) numerically, and computed the errors between the experimental and the simulation. The *Ode45* function of *MATLAB* was used to solve the differential equation by numerical integration using the fourth-order Runge-Kutta method. The parameter values were predicted using a genetic algorithm in *MATLAB* software. The algorithm can search for the optimal value of the process variable.[8] The reliability of the parameters was verified by minimising the error, *e*, between the experiment and the simulation, as shown in Fig. 1.

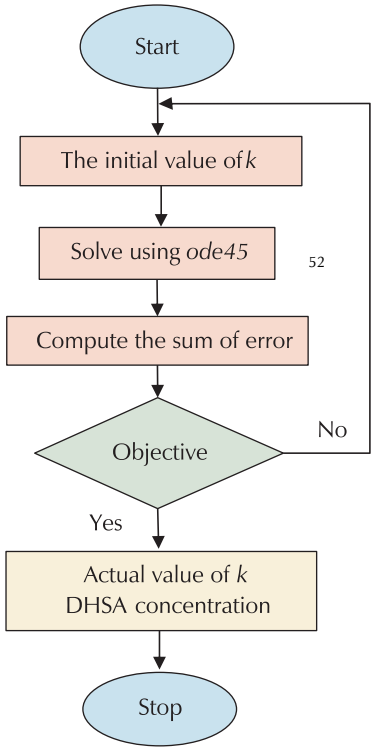

Fig. 1 – Determining reaction rate constant and optimisation of DHSA

2.2 Optimisation procedure

In recent research, the design of experiment (DOE) had been applied by implementing the Taguchi method approach. The method was developed by Taguchi and Kinoshito enhance the process parameters and increase the quality of components that were industrial.[9] This method employs a set of orthogonal arrays; with reaction parameters, optimisation is performed using the lowest possible number of experimental runs.[10] A few parameters, such as reaction temperature, FA to OA unsaturation molar ratio, H_2O_2 to OA unsaturation molar ratio, and agitation speed can affect the reaction of epoxidation. All these parameters were explored with the diversity of levels, as shown in Table 1. Therefore, the optimal reaction conditions of these vital reaction temperatures were analysed based on a DOE approach. The diversity of factors was studied by crossing the orthogonal array of the control parameters. The result obtained was further analysed manually using the signal to noise (S/N) ratio and analysis of variance (ANOVA). The optimum combination of reaction conditions projected by the Taguchi method was then tested and validated by running a confirmation reaction at the optimal predicted reaction conditions.

Table 1 – Design of experiment (DOE) using four parameters and three levels

Parameters		Levels		
		1	2	3
A	H_2O_2/OA unsaturation molar ratio	0.5	1	1.5
B	FA/OA unsaturation molar ratio	0.5	1	1.5
C	Temperature / °C	35	55	75
D	Agitation speed / rpm	100	200	300

Choosing the parameters was conducted according to the suggestion given by *D. B. Wijayasekara*.[11] For instance, 100 rpm, 200 rpm, and 300 rpm were the agitation speeds tested. The reaction temperatures (35, 55, 75 °C) were the reaction parameters, unsaturation molar ratio (0.5, 1.0, 1.5) of FA to OA, and unsaturation molar ratio (0.5, 1.0, 1.5) of H_2O_2 to OA, as shown in Table 1. Optimisation was conducted using the analytical Taguchi method to find the optimum conditions for every parameter.

3 Results and discussion

3.1 Reaction rate of DHSA production

Kinetic model for catalytic epoxidation of palm oleic acid based on palm oil (PO) was developed by *MATLAB* simulation. The kinetic data for the epoxidation and degradation of palm oil corresponded to the initial concentration. The Genetic Algorithm (GA) method was used to fit the experimental data and the Runge-Kutta fourth-order method was applied using the *Ode45* tool to solve the system of differential equations. There were 27 experiments run in the simulation, in order to ensure the optimal value of epoxidation. The experimental data was obtained from the previous experiments, and the simulation was based on that data. The initial concentration of formic acid (FA), hydrogen peroxide (H_2O_2), and oleic acid (OA) from previous experimental data was chosen as a reference to find the kinetic rate constant, *k*. On the other hand, the kinetic rate was used to determine the concentration of DHSA in oxirane cleavage. This occurred when the epoxide reacted with water. It corresponded to the objective of this study.

From the 27 experiments that were run (Table 2), experiment 11 was chosen as the best to display the optimised epoxidation process, as it had the lowest error (0.0937 %) compared to others. The reaction rate constants for this experiment were: k_{11} = 6.6442 mol l^{-1} min^{-1}, k_{12} = 11.0185 mol l^{-1} min^{-1}, k_{21} = 0.1026 mol l^{-1} min^{-1},

Table 2 – Simulation data

Exp	Initial concentration / mol l^{-1}			k_{11} / mol l^{-1} min^{-1}	k_{12} / mol l^{-1} min^{-1}	k_{21} / mol l^{-1} min^{-1}	k_{31} / mol l^{-1} min^{-1}	k_{41} / mol l^{-1} min^{-1}	k_{51} / mol l^{-1} min^{-1}	Error min	DHSA estimated concentration / mol l^{-1}
	H_2O_2	FA	OA								
1	1.4714	1.4714	2.9484	0.1174	0	0.0633	0.0135	0	0.0142	0.2945	0.733307
2	1.4714	1.4714	2.9484	0.1028	0	0.0470	0.0136	0	0.0166	0.2694	0.700095
3	1.4714	1.4714	2.9484	0.0543	0	8.5916	0.0283	0	0.0074	0.2892	1.017948
4	1.4714	2.9484	2.9484	6.0964	1.2061	0.0239	0.0094	0.0242	0.0131	0.1500	0.404717
5	1.4714	2.9484	2.9484	1.5720	1.9932	0.1575	0.0124	0	0.0075	0.3069	0.62633
6	1.4714	2.9484	2.9484	0.0691	0	0.1030	0.0100	0	0.0101	0.1412	0.482747
7	1.4714	4.4226	2.9484	0.0391	0	0.0967	0.0105	0	0.0068	0.1525	0.467893
8	1.4714	4.4226	2.9484	0.0299	0	0.0638	0.0077	0	0.005	0.2158	0.469234
9	1.4714	4.4226	2.9484	0.0477	0	0.1153	0.0078	0	0.0078	0.2258	0.360169
10	2.9484	1.4714	2.9484	6.4757	10.7925	0.0583	0.0171	0.0041	0.0161	0.1815	1.583085
11	**2.9484**	**1.4714**	**2.9484**	**6.6442**	**11.0185**	**0.1026**	**0.0238**	**0.0021**	**0.0142**	**0.0937**	**1.954907**
12	2.9484	1.4714	2.9484	12.8848	0	0.0251	0.0122	0	0.1811	0.1136	1.603342
13	2.9484	2.9484	2.9484	0.0486	0	0.0817	0.0168	0	0.0139	0.3010	1.592831
14	2.9484	2.9484	2.9484	0.0227	0	11.9431	0.0196	0	0.0058	0.1978	1.941024
15	2.9484	2.9484	2.9484	0.0505	0	0.1707	0.0147	0	0.0107	0.2550	1.626745
16	2.9484	4.4226	2.9484	0.3942	3.5703	0.0613	0.0135	0.0008	0.0059	0.1331	1.293596
17	2.9484	4.4226	2.9484	0.0342	2.8117	12.7116	0.0273	0.0203	0.0062	0.0723	1.37666
18	2.9484	4.4226	2.9484	1.1910	4.6865	0.0459	0.0106	0	0.0055	0.2295	1.33783
19	4.4226	1.4714	2.9484	1.5795	1.5004	0.0426	0.0203	0.0108	0.0205	0.1239	1.602207
20	4.4226	1.4714	2.9484	15	0	0.0495	0.0102	0.0365	0.1770	0.1532	1.759485
21	4.4226	1.4714	2.9484	4.6066	0.0925	0.0233	0.0101	0.0062	0.2219	0.3293	1.644378
22	4.4226	2.9484	2.9484	15	0	0.0128	0.0125	0	0.3158	0.1083	1.677388
23	4.4226	2.9484	2.9484	8.8191	1.6479	0.0231	0.0100	0.0033	0.0166	0.1530	1.719904
24	4.4226	2.9484	2.9484	12.1325	6.7678	14.3080	0.0036	9.1681	0.0003	0.2815	0.963317
25	4.4226	4.4226	2.9484	5.9174	0.1286	0.0272	0.0071	0.0226	0.0213	0.2420	1.208793
26	4.4226	4.4226	2.9484	0.0230	0	0.0573	0.0147	0	0.0073	0.1164	1.980805
27	4.4226	4.4226	2.9484	10.3146	0.6149	0.0414	0.0130	0.0261	0.0013	0.1213	2.482569

$k_{31} = 0.0238$ mol l^{-1} min^{-1}, $k_{41} = 0.0021$ mol l^{-1} min^{-1}, and $k_{51} = 0.0142$ mol l^{-1} min^{-1}. The concentration of DHSA obtained from this simulation was 1.954907 mol l^{-1}.

3.2 Optimisation of DHSA through Taguchi method

To determine the optimum reaction conditions for the production of DHSA, the Taguchi method was used, as presented in Table 3. Signal to noise (S/N) ratio is an analytical medium used to evaluate the most influential level of each factor that contributes to the optimum response value. L-27 orthogonal array with four factors and three levels for each factor was selected. The Taguchi orthogonal array experimental design is presented in Table 3, where the estimated concentration of DHSA was obtained from the simulation.

Table 3 – Taguchi orthogonal array experimental design for DHSA

Run	Reaction parameters and their levels				DHSA estimated concentration / mol l^{-1}
	Temperature /°C	FA/OA	H_2O_2/OA	Agitation speed / rpm	
1	1	1	1	1	0.733307
2	1	1	1	1	0.700095
3	1	1	1	1	1.017948
4	1	2	2	2	0.404717
5	1	2	2	2	0.626330
6	1	2	2	2	0.482747
7	1	3	3	3	0.467893
8	1	3	3	3	0.469234
9	1	3	3	3	0.360169
10	2	1	2	3	1.583085
11	2	1	2	3	1.954907
12	2	1	2	3	1.603342
13	2	2	3	1	1.592831
14	2	2	3	1	1.941024
15	2	2	3	1	1.626745
16	2	3	1	2	1.293596
17	2	3	1	2	1.376660
18	2	3	1	2	1.337830
19	3	1	3	2	1.602207
20	3	1	3	2	1.759485
21	3	1	3	2	1.644378
22	3	2	1	3	1.677388
23	3	2	1	3	1.719904
24	3	2	1	3	0.963317
25	3	3	2	1	1.208793
26	3	3	2	1	1.980805
27	3	3	2	1	2.482569

The "larger-the-better" S/N ratio indicated better performances regardless of the performance characteristics. According to the previous research,[6] the optimum level for all parameters would be the level with the greatest S/N ratio. The 27 experimental runs based on Taguchi method suggested that the optimum DHSA was obtained at H_2O_2/OA unsaturation molar ratio of 1 : 1 (level 2), FA/OA unsaturation molar ratio 0.5 : 1 (level 1), temperature of 35 °C (level 1), and agitation speed of 100 rpm (level 1). These results were plotted for each parameter in Fig. 2.

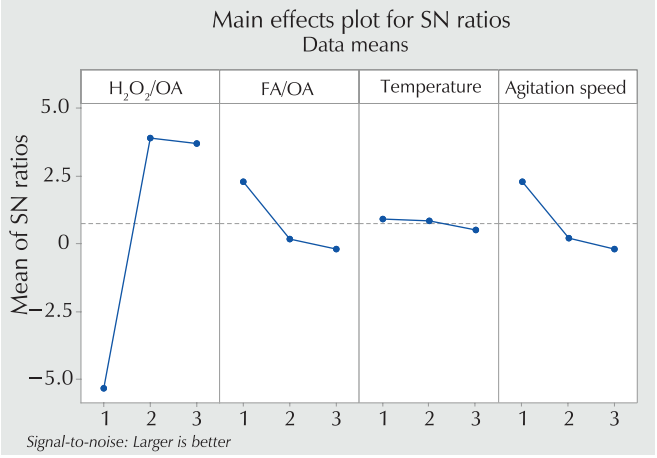

Fig. 2 – S/N Ratio for each level parameter affecting the DHSA yield

4 Conclusion

By developing the kinetic model of palm oil, it was found that the kinetic parameters were $k_{11} = 6.6442$ mol l^{-1} min^{-1}, $k_{12} = 11.0185$ mol l^{-1} min^{-1}, $k_{21} = 0.1026$ mol l^{-1} min^{-1} for epoxidation process, and $k_{31} = 0.0238$ mol l^{-1} min^{-1}, $k_{41} = 0.0021$ mol l^{-1} min^{-1}, $k_{51} = 0.0142$ mol l^{-1} min^{-1} in a degradation process. Furthermore, each of the reactions involved in the epoxidation and degradation process was successfully simulated in *MATLAB*. The minimum error for the simulation was about 0.0937 %. From the generated simulation, the data of DHSA yield in the reaction was obtained. Based on the chemical equation, the reactant will be used up, while the value of the concentration for the product will increase. Thus, the kinetic model was valid and the objective was achieved. The optimisation of DHSA yield was studied by the Taguchi method. The method resulted in the optimum value for producing DHSA based on the factors that had been decided, which were H_2O_2/OA unsaturation molar ratio of 1 : 1 (level 2), FA/OA unsaturation molar ratio 0.5 : 1 (level 1), temperature of 35 °C (level 1), and agitation speed of 100 rpm (level 1). From these values, the optimised value of DHSA can be achieved.

List of abbreviations

DEG 1 – degradation 1
DEG 2 – degradation 2
DHSA – dihydroxystearic acid
FA – formic acid
OA – oleic acid
EPO – epoxidized palm oil
PFA – performic acid
EPOXY – epoxidized oil
S/N – signal to noise

References

Literatura

1. "The Oil Palm Tree." [Online]. Available: https://www.palmoilhealth.org/what-is-palm-oil/the-oil-palm-tree/. [Accessed: 25-Nov-2018].
2. *M. J. Jalil, S. K. Jamaludin, A. Rafizan, M. Daud*, Degradation Oxirane Ring Kinetics of Epoxidized Palm Kernel Oil-Based Crude Oleic Acid, Ch&ChT **12** (3) (2018) 296–299, doi: https://doi.org/10.23939/chcht12.03.296.
3. *R. Guo, C. Ma, S. Sun*, Kinetic Study on Oxirane Cleavage of Epoxidized Palm Oil, JAOCS **88** (4) (2011) 517–521, doi: https://doi.org/10.1007/s11746-010-1697-4.
4. *C. Y. May, K. Nesaretnam*, Highlight Article Research advancements in palm oil nutrition, Eur. J. Lipid Sci. Technol. **116** (10) (2014) 1301–1315, doi: https://doi.org/10.1002/ejlt.201400076.
5. *Q. Ren, J. Pan, J. Zhou, Y. Na, C. Chen, W. Li*, Synthesis and Tribological Studies of Branched Alcohol Derived Epoxidized Synthesis and Tribological Studies of Branched Alcohol Derived Epoxidized Biodiesel, Materials **8** (10) (2015) 6623–6632, doi: https://doi.org/10.3390/ma8105326.
6. *R. Ismail, R. Awang, A. H. Hazimah*, Palm dihydroxystearic acid (DHSA): A multifunctional ingredient for various applications, J. Oil Palm Res. **27** (3) (2015) 195–211, url: http://jopr.mpob.gov.my/wp-content/uploads/2015/09/jopr v27sept-rosnah1.pdf.
7. *G. Koay, A. L. Chuah, R. Yunus, P. Siwayanan*, Crystallization of dihydroxystearic acid (DHSA) produced from commercial grade palm oil based crude oleic acid employing isopropyl alcohol as solvent, Int. J. Eng. Technol. **3** (1) (2006) 115–124.
8. *K. S. Prasad, C. S. Rao, D. N. Rao*, Study on Factors Effecting Weld Pool Geometry of Pulsed Current Micro Plasma Arc Welded AISI 304L Austenitic Stainless Steel Sheets Using Statistical Approach, J. Miner. Mater. Charact. Eng. **11** (8) (2012)790–799, doi: https://doi.org/10.4236/jmmce.2012.118068.
9. *S. Athreya, Y. D. Venkatesh*, Application of Taguchi Method for Optimization of Process Parameters in Improving the Surface Roughness of Lathe Facing Operation, IRJES **1** (3) (2012) 13–19, url: http://irjes.com/Papers/vol1-issue3/Version%201/C131319.pdf.
10. *A. Martínez-Vargas*, Optimizing grade-control drillhole spacing with conditional simulation, **33** (2017) 1–12, url: http://scielo.sld.cu/pdf/mg/v33n1/mg01117.pdf.
11. *D. B. Wijayasekara*, Minimum Agitation Speed for Solid Suspension and Mixing Time in a Torispherical-Bottomed Pharmaceutical Stirred Tank Under Different Baffling Conditions, MSc Thesis, p. 125, 2007.

SAŽETAK

Dihidroksistearinska kiselina (DHSA) visokog prinosa temeljena na kinetičkom modelu iz epoksidiranog palmina ulja

Mohd Jumain Jalil,[a*] *Khairul Azhar Kamal*,[a] *Aliff Farhan Bin Mohd Yamin*,[a] *Intan Suhada Azmi*,[b] *Mohamad Hasni Hassan*,[a] *Abdul Rani Hidayu*[b] i *Kamariah Noor Ismail*[c]

Posljednjih godina studije povezane s epoksidacijom masnih kiselina izazvale su veliko zanimanje zbog sve veće potražnje za ekološki prihvatljivim epoksidima dobivenim iz biljnih ulja. Iz reakcije epoksidacije dolazi do nuspojave koja uključuje epoksid i vodu. Tom reakcijom nastaje nusproizvod – dihidroksistearinska kiselina (DHSA). DHSA jedan je od kemijskih prekursora u proizvodnji kozmetičkih proizvoda. Stoga je razvijen kinetički model za određivanje optimiranog procesa epoksidacije i koncentracije DHSA, gdje je identificirana svaka od reakcija. Dobiveni parametri kinetičke brzine, k bili su: k_{11} = 6,6442, k_{12} = 11,0185, k_{21} = 0,1026 za epoksidacijsku palmino-oleinsku kiselinu i k_{41} = 0,0021, k_{51} = 0,0142 u procesu razgradnje. Minimalna pogreška simulacije bila je 0,0937. Uz to, optimizacija prinosa DHSA provedena je Taguchijevom metodom, a dobiveni optimalni uvjeti su molarni omjer nezasićenja H_2O_2/oleinske kiseline – OA 1 : 1 (razina 2), molarni omjer nezasićenja mravlje kiseline – FA/OA 0,5 : 1 (razina 1), temperatura 35 °C (razina 1) i brzina miješanja 100 o min^{-1} (razina 1). Pod tim se uvjetima može postići visok prinos DHSA.

Ključne riječi
Epoksidacija, kinetika, MATLAB, DHSA, Taguchi

[a] *Faculty of Chemical Engineering, Universiti Teknologi MARA Cawangan Pulau Pinang, Kampus Permatang Puah, 13 500 Permatang Pauh, Pulau Pinang*
[b] *Faculty of Chemical Engineering, Universiti Teknologi Mara Cawangan Johor Kampus Pasir Gudang, 81 750 Masai, Johor*
[c] *Faculty of Chemical Engineering, Universiti Teknologi MARA, 40 450 Shah Alam, Selangor*

Izvorni znanstveni rad
Prispjelo 30. ožujka 2020.
Prihvaćeno 27. srpnja 2020.