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Dihydroxystearic Acid Production *via* Catalytic Epoxidation of Oleic Acid Derived from Palm Oil

I. M. Rasib,[a] *I. S. Azmi,*[a] *M. `A. Addli,*[a] *F. Fitriana,*[b]
A. N. Masri,[c] and *M. J. Jalil*[a*]

[a] Faculty of Chemical Engineering, Universiti Teknologi MARA, Cawangan Johor, Kampus Pasir Gudang, 81 750 Masai Johor, Malaysia
[b] Universitas Negeri Surabaya, Indonesia
[c] Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81 310 Johor Bahru, Johor, Malaysia

Abstract

Concern regarding the drawbacks of relying on fossil fuels as the primary resource for producing various derivatives has led to increased interest in the production of dihydroxystearic acid (DHSA) *via in situ* hydrolysis of epoxidised oleic acid. Epoxidised oleic acid is produced using *in situ* formed performic acid (HCOOOH), a mixture of formic acid (HCOOH) as the oxygen carrier and hydrogen peroxide (H_2O_2) as the oxygen donor. A genetic algorithm method implemented in MATLAB was used to simulate the kinetics of oxirane oxygen ring degradation during the epoxidation process, along with the concentration of DHSA produced. This approach is novel in combining the genetic algorithm with the Runge-Kutta method, providing more accurate and efficient kinetic modelling than conventional methods. The DHSA produced, known as crude DHSA, was further purified for potential application in the cosmetics industry.

The physicochemical properties of both crude and purified DHSA were compared. The hydroxyl value for the purified DHSA was higher (333.1 mg KOH/g) compared to that of the crude (267 mg KOH/g). Other properties, such as higher iodine value in the crude (8.9) compared to purified (3.7), were also confirmed. Additionally, the most significant difference observed was in the form or particle size: crude DHSA appeared as a semi-solid, whereas purified DHSA was a white powder with a particle size range of 63–125 µm.

Keywords

Epoxidation, DHSA, ode45, biomass conversion

1 Introduction

Concerns over fossil fuel supply, carbon emissions, and rising petroleum costs highlight the need for alternative energy sources.[1] In addition, new environmental regulations and societal concerns have triggered the search for more environmentally friendly alternatives.[2] Vegetable oils are among the most favourable renewable resources due to their sustainability and lower pollutant emissions.[3] Approximately 50 % of palm oil is made up of unsaturated fatty acids, of which 40 % is oleic acid with the remaining 10 % comprising a combination of polyunsaturated linoleic and linolenic acids.[4] The highest lipid content of oleic and linoleic acids among all the fatty acids makes them suitable for further processing into raw materials for the production of skincare products.[5] Epoxidation converts unsaturated fatty acids into reactive groups useful in the synthesis of chemicals and polymers like polyesters, polyurethanes, and epoxy resins.[6]

Under acidic conditions, the epoxides have a high tendency to undergo epoxide cleavage or epoxide ring degradation, initiated by either electrophiles or nucleophiles.[7] Epoxides themselves act as intermediates in the synthesis of various chemicals.[8] The epoxidation process involves two steps, as shown in Fig. 1.[9]

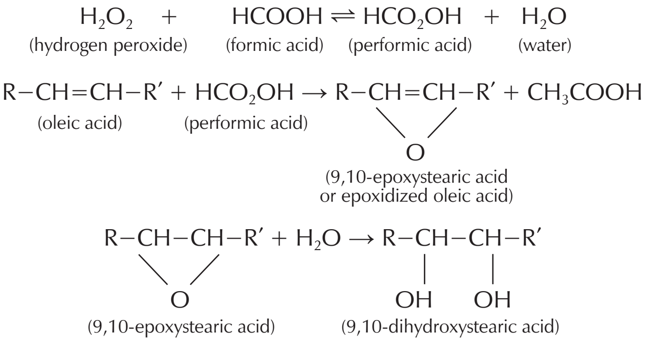

Fig. 1 – Schematic of epoxidation and oxirane ring opening

The proposed method presents several limitations that make it less favourable. Firstly, it would require the repetition of all 27 experimental runs, with each run lasting 2 h. The crude DHSA obtained from each experiment would then need to be analysed using Fourier transform infrared (FTIR) spectroscopy and hydroxyl value analysis to confirm product formation. This process is not only time-consuming but also inefficient. Secondly, the cumulative reaction time of approximately 57 h renders the method impractical, as it would lead to excessive consumption of chemicals and resources. These drawbacks highlight the need for a more streamlined and resource-efficient approach. To ad-

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

dress this, a process model for DHSA production *via in situ* hydrolysis of epoxidised oleic acid was developed using MATLAB to determine the reaction kinetics and estimate DHSA concentration based on data from 27 previously conducted experiments.[10] At present, there are limited studies on the production of DHSA using *in situ* hydrolysis of epoxidised oleic acid under optimised epoxidation process parameters. This is due to the limited availability of palm oil in many countries compared to Malaysia. Although several studies have focused on optimising epoxidation parameters for oils such as *Hura crepitans* seed oil,[11] rapeseed oil,[12] and cottonseed oil,[13] fewer have investigated oxirane ring-opening in epoxidised palm oil. Considering that optimised epoxidation process parameters can yield crude DHSA through *in situ* hydrolysis of epoxidised oleic acid, a high hydroxyl content would be produced, indicative of high DHSA yield. DHSA is a potential chemical modification of oxirane ring structure from oleic acid epoxidation following hydrolysis.[14] However, limited studies have explored the purification of crude DHSA from epoxidised oleic acid, necessitating further research for detailed characterisation. Purification yields a form of DHSA suitable for use as a cosmetic raw material. Consequently, the value of DHSA can be increased, making it more marketable within the industry. This study introduces a novel approach to the production of dihydroxystearic acid from the catalytic epoxidation of oleic acid derived from palm oil, leveraging an innovative reaction pathway. This research aimed to develop a kinetic model for the catalytic epoxidation of palm oleic acid using MATLAB and to analyse the physicochemical properties of both crude and purified DHSA. The novelty of this study lies in the efficient *in situ* generation of peracids, enabling selective epoxidation of oleic acid, followed by controlled ring opening to produce DHSA. By employing a tailored catalytic system, this process enhances reaction efficiency, minimises side reactions, and ensures high product purity. This method not only offers a sustainable and scalable route for DHSA production but also aligns with green chemistry principles by utilising renewable palm oil as a feedstock and reducing reliance on hazardous chemicals. Furthermore, this study introduces a hybrid modelling approach that integrates the 4th-Order Runge-Kutta method with a genetic algorithm to accurately simulate the kinetics of oleic acid epoxidation. This offers improved parameter estimation and predictive capability compared to traditional methods. Additionally, the work demonstrates the selective production of dihydroxystearic acid from palm oil-derived oleic acid, contributing to the advancement of sustainable, bio-based chemical processes.

2 Materials and method

Palm oleic acid, HCOOH, H_2O_2, H_2SO_4, and acetic acid were purchased from Merck Sdn. Bhd. and QReC Sdn. Bhd. (Table 1).

Table 1 – List of chemicals used for the production of crude DHSA

Materials	Range/Amount	Purity/Molarity	Supplier
Oleic acid	100 g	75 %	QReC Sdn. Bhd.
HCOOH	1.0	23.6 M	QReC Sdn. Bhd.
H_2O_2	1.0	50 %	Merck Sdn. Bhd.
H_2SO_4	0.2 g	18.0 M	QReC Sdn. Bhd.
Acetic acid	5 ml	12 M	QReC Sdn. Bhd

2.1 Experimental setup

The epoxidation was conducted in a 500 ml beaker with a hot plate as the heat source. Oleic acid (100 g) was mixed with HCOOH (0.5 molar ratio) and stirred at 200 rpm in a thermostatic water bath maintained at 35 °C. Hydrogen peroxide (H_2O_2) at a 1.5 molar ratio was added dropwise to the mixture, followed by 2 g of H_2SO_4 catalyst. The reaction ran for 2 h. Samples of 3 g were collected every 5 min for the first 30 min to analyse oxirane content, following the AOCS Cd-957 method. The oxygen oxygen content (OOC) of each sample was determined and used to calculate the relative conversion to oxirane (RCO). Samples with the highest OOC were selected for physicochemical analysis to confirm the characteristics of the epoxidised oleic acid. After 2 h, the crude DHSA formed was collected for physicochemical characterisation to verify its DHSA characteristic and to undergo further purification to reduce its skin irritancy, thereby making it suitable for cosmetic applications. Samples of crude DHSA were collected after the two-hour *in situ* hydrolysis process, as at this point the epoxidised oleic acid and OOC were fully converted into crude DHSA.

2.2 Purification of crude DHSA

Crude DHSA was further purified to remove its acidity, which may cause skin irritation, thus making it suitable for use in cosmetic products. The purification process consisted of three main steps: 1) Recrystallisation from solvent: a mixture of isopropanol and in an 80:20 ratio was prepared. This was combined in a 1 : 1 ratio with crude DHSA and kept at 5 °C for 3 days to allow crystallisation. 2) Solvent removal: the purified DHSA crystals in wet form were filtered through fine-pore cloth to remove excess isopropanol and water mixture. The crystals were then thoroughly washed with water. 3) Drying: the washed purified DHSA crystals were dried under sunlight to remove any remaining moisture. The purified DHSA was then characterised by hydroxyl value, water content, iodine value, acidity value, and sieve analysis.[10]

2.3 Relative conversion to oxirane (RCO)

The relative conversion to oxirane is a key parameter used to assess the efficiency and selectivity of the epoxidation reaction.[15] Eq. (1) is based on the oxirane oxygen content (OOC) value, determined theoretically (Eq. (2)) and experimentally (Eq. (3)).

$$\mathrm{RCO} = \frac{\mathrm{OOC_{exp}}}{\mathrm{OOC_{theor}}} \cdot 100 \tag{1}$$

$$\mathrm{OOC_{theo}} = \left\{ \left(\frac{X_0}{A_i}\right) / \left[100 + \frac{X_0}{2A_i} \cdot A_\mathrm{o} \right] \right\} \cdot A_\mathrm{o} \cdot 100 \tag{2}$$

$$\mathrm{OOC_{exp}} = 1.6 \cdot N \cdot \frac{V - B}{W} \tag{3}$$

where, X_0 is the initial iodine value, A_i is the molar mass of iodine, A_o is the molar mass of oxygen, N is the normality of HBr, V is the volume of the HBr solution used for the blank in milliliters (ml), B is the volume of HBr solution used for titration, and W is the weight of the sample.

2.4 Hydroxyl value

The hydroxyl value (*OHV*) is a measure of the number of hydroxyl (OH) groups present in a sample of a material, such as a polyol, alcohol, or polymer. The hydroxyl value is a useful tool for characterising and comparing different DHSA products, and is widely used in the chemical industry. The hydroxyl value can be determined using Eq. (4).

$$OHV \left[\frac{\mathrm{mg\ KOH}}{\mathrm{g}}\right] = \frac{\left(B - EQ_1\right) \cdot T \cdot M \cdot F_1}{W \cdot F_2} \tag{4}$$

B is the blank value, EQ_1 is titrant consumption at the first equivalence point, T is titrant concentration, M is molecular weight, W is sample weight (g), and F_1 and F_2 are conversion factors.

2.5 Kinetic model of degradation of epoxidized oleic acid

To establish the experimental procedure for the production of crude DHSA, it is necessary to develop both the reaction rate (k) and the concentration of crude DHSA. This step addresses the first objective of this study. Data from 27 previously conducted experiments involving the determination of RCO – also known as the epoxy ring opening – are presented in Table 2. The RCO values reflect the structural transformation of epoxidised oleic acid into crude DHSA.

The kinetic study, aimed at determining the rate constant for each reaction is presented in Eqs. (5)–(7). In these equa-

Table 1 – Data from 27 previous experiments of epoxidised oleic acid[10]

No. exp.	H_2O_2/Oleic acid	HCOOH/oleic acid	Temp / °C	Catalyst	RPM	$\mathrm{OOC_{exp}}$
1	0.5	0.5	35	H_2SO_4	100	1.20
2	0.5	0.5	35	H_2SO_4	200	1.26
3	0.5	0.5	35	H_2SO_4	300	1.33
4	0.5	1	35	H_2SO_4	100	0.79
5	0.5	1	55	HCL	200	1.45
6	0.5	1	55	HCL	300	1.08
7	0.5	1.5	75	HCL	100	1.13
8	0.5	1.5	75	HNO_3	300	1.31
9	0.5	1.5	75	HNO_3	300	1.19
10	1	0.5	55	HNO_3	100	1.16
11	1	0.5	55	HNO_3	200	1.19
12	1	0.5	55	HNO_3	300	1.29
13	1	1	75	H_2SO_4	100	1.45
14	1	1	75	H_2SO_4	200	1.56
15	1	1	75	H_2SO_4	300	1.60
16	1	1.5	35	H_2SO_4	100	1.03
17	1	1.5	35	H_2SO_4	200	1.09
18	1	1.5	35	HCl	300	1.35
19	1.5	0.5	75	HCl	100	0.94
20	1.5	0.5	75	HCl	200	1.33
21	1.5	0.5	75	HCl	300	1.05

Table 1 – (continued)

No. exp.	H_2O_2/Oleic acid	HCOOH/oleic acid	Temp / °C	Catalyst	RPM	OOC_{exp}
22	1.5	1	35	HNO_3	100	1.08
23	1.5	1	35	HNO_3	200	1.29
24	1.5	1	35	HNO_3	300	1.41
25	1.5	1.5	55	H_2SO_4	100	1.38
26	1.5	1.5	55	H_2SO_4	200	1.34
27	1.5	1.5	55	H_2SO_4	300	1.44

tions, A, B, C, epoxide, and D represent formic acid, hydrogen peroxide, performic acid, epoxidised palm oleic acid, and crude DHSA, respectively. Eqs. (5) and (6) describe the epoxidation process, while Eq. (7) represents the formation of crude DHSA *via in situ* hydrolysis, during which the epoxidised oleic acid undergoes oxirane ring opening to form crude DHSA. The kinetic model developed for DHSA production is based on several simplifying assumptions that may limit its applicability under complex or industrial-scale conditions. The model does not explicitly account for mass transfer effects, catalyst deactivation, or the influence of side reactions such as hydrolysis and ring-opening under varying operational parameters. Additionally, the use of average experimental conditions may obscure local variations in concentration and temperature. This model assumes the following: (1) a single-phase epoxidation process, (2) constant phase volume, (3) homogeneous reactions, and (4) reactions occurring away from the interface. The epoxidation of oleic acid was modelled using a system of ordinary differential equations (ODEs) representing both epoxide formation and side reactions. These equations were solved using the Runge-Kutta fourth-order (RK4) method, while the kinetic parameters were estimated *via* a genetic algorithm (GA) by minimising the error between the simulated and experimental data. This combined RK4-GA approach provides an accurate method for kinetic modelling and facilitates effective process optimisation.

$$A + B \underset{k_{12}}{\overset{k_{11}}{\rightleftarrows}} C + H_2O \tag{5}$$

$$C + \text{oleic acid} \xrightarrow{k_2} \text{epoxide} + A \tag{6}$$

$$\text{epoxide} + H_2O \xrightarrow{k_3} \text{DHSA} \tag{7}$$

The rate equations were simultaneous differential equations, and are presented in Eqs. (8)–(13).

$$\frac{d[A]}{dt} = -k_{11}[A][B] + k_{12}[C][H_2O] + k_2[C][\text{oleic acid}] \tag{8}$$

$$\frac{d[B]}{dt} = -k_{11}[A][B] + k_{12}[C][H_2O] \tag{9}$$

$$\frac{d[C]}{dt} = k_{11}[A][B] - k_{12}[C][H_2O] - k_{21}[C][\text{oleic acid}] \tag{10}$$

$$\frac{d[\text{oleic acid}]}{dt} = -k_2[C][\text{oleic acid}] \tag{11}$$

$$\frac{d[\text{epoxide}]}{dt} = k_{21}[C][\text{oleic acid}] - \\ -k_{22}[\text{epoxide}][A] - k_3[\text{epoxide}][H_2O] \tag{12}$$

$$\frac{d[\text{DHSA}]}{dt} = k_3[\text{epoxide}][H_2O] \tag{13}$$

Parameter reliability was verified by minimising the error between simulation and experimental results, defined in Eq. (14).

$$\text{Error} = \sum_{i=1}^{n} \frac{\left|\text{DHSA}_i^{\text{sim}} - \text{DHSA}_i^{\text{exp}}\right|}{n} \tag{14}$$

$\text{DHSA}_i^{\text{sim}}$ and $\text{DHSA}_i^{\text{exp}}$ denote the estimated and experimental epoxy concentrations, *i* is the *i*th data point, and *n* is the total number of data points in the simulations and experiments.

3 Results and discussion

3.1 Kinetic model for the degradation of epoxidised oleic acid

To establish an experimental procedure for the production of crude DHSA, it is essential to develop both the reaction rate (*k*) and the concentration of crude DHSA. Data from 27 previous experiments involving determining the relative conversion oxirane (also known as the epoxide ring opening) are presented in Table 3. This relative conversion reflects the structural transformation of epoxidised oleic acid into DHSA.

Table 3 – Data from 27 previous experiments of epoxidised oleic acid where oxirane oxygen content data was used to estimate kinetic rate[10]

No.	k_{11}	k_{12}	k_2	k_3	DHSA	Error
1	3.34	5.55	0.08	0.04	2.83	0.22
2	0.0896	$1.7689 \cdot 10^{-7}$	0.11	0.04	1.41	0.21
3	6.57	10.05	0.09	0.039	1.40	0.31
4	0.032	$3.02 \cdot 10^{-8}$	0.08	0.08	1.44	0.15
5	2.16	23.28	0.09	0.07	1.43	0.17
6	2.13	18.57	0.08	0.07	1.43	0.17
7	0.07	14.74	3.92	0.04	1.41	0.21
8	0.04	$5.62 \cdot 10^{-8}$	0.17	0.04	1.41	0.18
9	2.80	21.28	0.17	0.04	1.41	0.21
10	0.08	$2.84 \cdot 10^{-7}$	0.11	0.06	2.87	0.18
11	0.08	$1.32 \cdot 10^{-8}$	0.11	0.06	2.87	0.18
12	0.08	$3.06 \cdot 10^{-8}$	0.11	0.06	2.87	0.18
13	0.03	$1.32 \cdot 10^{-7}$	0.10	0.06	2.87	0.18
14	0.03	$1.22 \cdot 10^{-9}$	0.10	0.06	2.87	0.18
15	3.89	24.95	0.12	0.06	2.85	0.21
16	0.02	$3.88 \cdot 10^{-8}$	0.10	0.06	2.87	0.17
17	1.93	18.89	0.12	0.06	2.85	0.21
18	0.02	$1.36 \cdot 10^{-8}$	0.10	0.06	2.87	0.17
19	0.04	$1.83 \cdot 10^{-8}$	0.14	0.06	2.95	0.14
20	8.30	4.47	0.05	0.04	2.95	0.18
21	2.17	19.12	0.18	0.07	2.95	0.21
22	0.02	$1.33 \cdot 10^{-8}$	0.08	0.05	2.95	0.13
23	0.83	4.84	0.09	0.06	2.95	0.19
24	2.26	19.39	0.08	0.05	2.95	0.20
25	8.65	8.68	0.03	0.03	2.95	0.19
26	2.60	18.42	0.07	0.05	2.95	0.20
27	3.26	18.05	0.07	0.05	2.95	0.19

3.2 DHSA production form optimised epoxidised oleic acid

This study focuses on the optimisation of DHSA production by systematically exploring and enhancing the transformation of epoxidised oleic acid. DHSA, a valuable precursor in various industrial applications, is derived from epoxidised oleic acid through controlled hydrolysis and subsequent processing. The objective was to improve both the efficiency and yield of DHSA production by employing optimisation strategies, including reaction conditions and catalyst selection. The degradation phase corresponds with the hydrolysis period, during which epoxidised oleic acid undergoes a series of chemical transformations that lead to the formation of DHSA. Fig. 2 illustrates the dynamic behaviour of the epoxidised oleic acid hydrolysis process under optimised reaction conditions, with a focus on the percentage of remaining epoxidised oleic acid (RCO) over

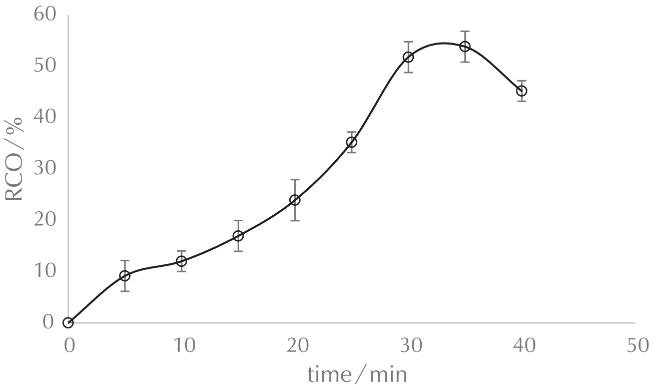

Fig. 2 – DHSA production *via in situ* epoxidation of oleic acid

time. The optimised conditions result in a peak RCO percentage of 55 %, indicating the highest achievable conversion of epoxidised oleic acid. This indicates successful utilisation of the optimised conditions for maximising the production of DHSA. Beyond the peak conversion, the RCO percentage starts to degrade after approximately 35 min. This degradation phase coincides with the onset of hydrolysis for DHSA formation. The decreasing RCO percentage suggests the ongoing transformation of epoxidised oleic acid into DHSA.

3.3 Comparison of hydroxyl value of crude and pure DHSA

An isopropanol-water solution was used to purify crude DHSA. The hydroxyl value of purified DHSA increased as the viscosity of crude DHSA decreased, with water acting as an agglomerating agent that facilitated the formation of fine purified DHSA particles.[18] The hydroxyl value is defined as the number of milligrams of potassium hydroxide required to neutralise the acetic acid derived from one gram of a chemical substance containing free hydroxyl groups. An increase in hydroxyl groups from crude to purified DHSA is crucial for enhancing various characteristics useful in cosmetic products, such as nullifying its dermal irritancy caused by residual acidity from H_2O_2 and HCOOH at the beginning of production, as well as enhancing its stick-forming ability for deodorants and glossiness for lipsticks. According to *Rosnah et al.*,[19] the purification of crude DHSA to purified DHSA showed a significant improvement in the hydroxyl value from 220.7 to 357.6 mg KOH/g. After purification, the hydroxyl value increased from 221.8 mg KOH/g for crude DHSA to 333.1 mg KOH/g for purified DHSA. This confirms the success of the purification process, as the objective was to produce purified DHSA with a higher hydroxyl value than the crude DHSA. A high hydroxyl value indicates greater reactivity, enabling faster and more effective reactions. It also enhances solubility in specific solvents, making them easier to handle during the production of cosmetic products. Fig. 3 presents the comparison of the hydroxyl values of crude and purified DHSA.

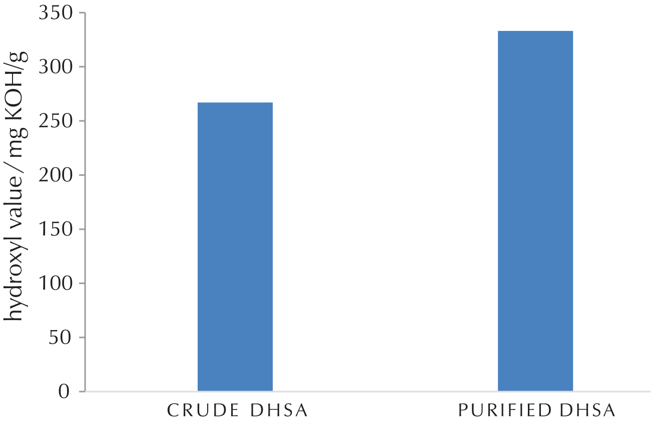

Fig. 3 – Hydroxyl values of crude and purified DHSA

3.4 Physicochemical properties

Several physicochemical properties need to be analysed to verify the successful purification of crude DHSA. The key properties involved include hydroxyl value, moisture content, particle size, iodine value, and acid value. Iodine value measures the amount of unsaturated fat in a compound, expressed as the amount of iodine absorbed.[20] The iodine value test performed for both crude and purified DHSA showed a decrease in iodine value, indicating the conversion of the double bond of carbon in crude DHSA to a more saturated compound, or the formation of the chain of saturated fatty acid.

Moisture content determines the weight of water in a sample. In order to produce deodorant sticks, it is important for purified DHSA to have a low water content because a high-water content would disturb the blending with humectants, perfume, and antimicrobial agents. The purified DHSA has a lower moisture content than crude DHSA, as per other researchers.[21] Crude DHSA is a white semi-solid material due to unreacted excess acid during the hydrolysis process along with water. Hence, after purification, a white crystalline structure was produced, and it was then sieved to determine the particle size. Table 4 presents the results of the physicochemical properties of crude and purified DHSA. While DHSA has been reported in the literature as a promising compound for applications in the cosmetic industry, the present study focuses solely on its production *via* the selected synthetic route. Comprehensive assessments relating to product purity, safety, and regulatory compliance, and critical parameters for cosmetic applications were beyond the scope of this work. Future research should aim to assess the physicochemical properties, toxicological profile, and formulation compatibility of DHSA to determine its suitability in line with industry standards.

Table 4 – Physicochemical properties of crude and purified DHSA

Test description	Unit	Crude DHSA	Purified DHSA
Iodine value	–	8.9	3.7
Acid value	mg KOH/g	160.4	172.6
Moisture content	%w/w	0.93	0.17
Form/particle size	µ	semi-solid	63–125

4 Conclusion

Following the successful formation of crude DHSA, a purification step was carried out, and the physicochemical properties of both crude and purified DHSA were determined and compared. The hydroxyl value of purified DHSA was higher than that of crude DHSA, measured at 333.1 and 267 mg KOH/g, respectively. Other properties include higher iodine value in crude DHSA (8.9) compared to purified DHSA (3.7), and the form or particle size which show the most significant properties where crude DHSA appears as a semi solid while purified DHSA is a white powder with particle size of 125–63 µm.

Overall, purified DHSA can be produced *via in situ* hydrolysis of epoxidised oleic acid by applying the rate reaction, *k*, and optimum parameter by *ode45* MATLAB simulation and Taguchi method, respectively. The purified DHSA obtained at the end of this study demonstrates suitable characteristics for potential application in cosmetics related industries.

Ethics approval

Not applicable.

Competing interests

The authors declare no competing interests

Author contribution

Ismail Md Rasib: Writing and experiment work; Fitriana Fb: Writing; Asiah Nusaibah Masri: Writing; Intan Suhada Azmi: Data curation; Mohd Jumain Jalil: conceptualization and methodology.

Availability of data and materials

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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SAŽETAK

Proizvodnja dihidroksistearinske kiseline katalitičkom epoksidacijom oleinske kiseline dobivene iz palmina ulja

Ismail Md Rasib,[a] *Intan Suhada Azmi*,[a] *Mohammad `Aathif Addli*,[a] *Fitriana Fitriana*,[b]
Asiah Nusaibah Masri,[c] and *Mohd Jumain Jalil* [a*]

Zabrinutost zbog prevelikog oslanjanja na fosilna goriva kao primarnog izvora za proizvodnju raznih derivata potaknula je veće zanimanje za sintezu dihidroksistearinske kiseline (DHSA) putem *in situ* hidrolize epoksidirane oleinske kiseline. Epoksidirana oleinska kiselina dobiva se uporabom *in situ* tvorene performične kiseline (HCOOOH), nastalom iz smjese mravlje kiseline (HCOOH) kao nosača kisika i vodikova peroksida (H_2O_2) kao donora kisika. Za simulaciju kinetike razgradnje oksiranskog (epoksidnog) prstena tijekom procesa epoksidacije, kao i koncentracije nastalog DHSA, primijenjena je metoda genetičkog algoritma implementirana u MATLAB-u. Taj pristup je nov po kombiniranju genetičkog algoritma s metodom Runge–Kutta, čime se postiže točnije i učinkovitije kinetičko modeliranje u odnosu na konvencionalne metode. Dobiveni DHSA, tzv. sirovi DHSA (*crude DHSA*), dodatno je pročišćen radi potencijalne primjene u kozmetičkoj industriji. Uspoređena su fizikalno-kemijska svojstva sirovog i pročišćenog DHSA. Hidroksilni broj pročišćenog uzorka bio je viši (333,1 mg KOH/g) u odnosu na sirovi (267 mg KOH/g). Također je potvrđena razlika u drugim svojstvima, primjerice jodni broj bio je veći kod sirovog uzorka (8,9) nego kod pročišćenog (3,7). Najizraženija razlika opažena je u obliku/veličini čestica: sirovi DHSA bio je polučvrst, dok je pročišćeni DHSA bio bijeli prah s rasponom veličina čestica 63–125 µm.

Ključne riječi
Epoksidacija, DHSA, ode45, konverzija biomase

[a] *Faculty of Chemical Engineering, Universiti Teknologi MARA, Cawangan Johor, Kampus Pasir Gudang, 81 750 Masai Johor, Malezija*
[b] *Universitas Negeri Surabaya, Indonezija*
[c] *Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia, 81 310 Johor Bahru, Johor, Malezija*

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