JPPIPA 12(6) (2026)

Jurnal Penelitian Pendidikan IPA

http://jppipa.unram.ac.id/index.php/jppipa/index

Optimized Coconut Oil-Derived Methyl Ester Sulfonate with Enhanced Detergency and Biodegradability for Liquid Detergent Applications

Syamsuddin[1*], Jusman[1]

[1] Faculty of Mathematics and Natural Sciences, University of Tadulako, Palu, Indonesia.

Received: July 10, 2024
Revised: January 21, 2026
Accepted: June 06, 2026
Published: June 30, 2026

Corresponding Author:
Syamsuddin
syamsuddinpalu2023@gmail.com

DOI: 10.29303/jppipa.v12i6.8474

Abstract: Methyl ester sulfonate (MES) is a renewable anionic surfactant with potential applications in sustainable liquid detergent systems. This study developed an integrated feedstock–process–structure–performance–degradation framework for the experimental production of coconut-oil-derived MES. Coconut oil quality and fatty acid methyl ester (FAME) reproducibility were evaluated prior to MES synthesis optimization using a three-factor Box–Behnken design. The effects of sulfonating-agent-to-FAME molar ratio, reaction temperature, and aging time were evaluated based on active MES content, residual FAME, disalt content, color, critical micelle concentration, surface tension, detergency, biodegradation, and liquid-detergent performance. Multiresponse optimization identified the optimum sulfonation condition at a sulfonating-agent-to-FAME molar ratio of 1.180, reaction temperature of 81.2 °C, and aging time of 67 min, with an overall desirability value of 0.709. Five independent experimental validation batches produced 85.8% active MES, 5.2% residual FAME, 5.7% disalt, a critical micelle concentration of 0.81 mM, minimum surface tension of 31.3 mN m^{-1}, detergency of 77.2%, and 82.3% biodegradation after 28 days. The optimized MES demonstrated competitive cleaning performance toward lipid-based soils under hard-water conditions and showed improved interfacial and environmental properties compared with the over-sulfonated product. In a 12% active liquid-detergent formulation, the all-MES system achieved 80.4% detergency, comparable with the sodium laureth sulfate reference formulation (81.2%), while the MES/SLES blend achieved 82.5% detergency. Excessive sulfonation reduced product quality by increasing secondary-product formation, decreasing interfacial efficiency, and negatively affecting biodegradation performance. Overall, balanced sulfonation optimization is essential for achieving MES with desirable chemical quality, application performance, and environmental compatibility. This framework provides a basis for further pilot-scale development of coconut-oil-derived MES as a renewable surfactant for liquid detergent applications.

Keywords: Anionic surfactant; Biodegradability; Coconut oil; Detergency; Liquid detergent; Methyl ester sulfonate; Response surface methodology

Introduction

Surfactants are essential components of household and industrial detergent systems because they reduce interfacial tension, improve wetting, disperse oily soils, stabilize emulsions, and minimize soil redeposition. Their performance is determined by interactions among molecular structure, critical micelle concentration, water hardness, temperature, soil characteristics, and formulation components. Therefore, detergency is recognized as a system-level property rather than a direct consequence of low surface tension or high foam generation alone (Danov et al., 2021; Lynn et al., 2020; Vega et al., 2025; Yavrukova et al., 2020)

The development of renewable surfactants has received increasing attention due to concerns regarding

How to Cite:
Syamsuddin, S., & Jusman, J. (2026). Optimized Coconut Oil-Derived Methyl Ester Sulfonate with Enhanced Detergency and Biodegradability for Liquid Detergent Applications. *Jurnal Penelitian Pendidikan IPA*, *12*(6), 732–739. https://doi.org/10.29303/jppipa.v12i6.8474

fossil-resource dependence and environmental impacts associated with conventional petrochemical surfactants. However, renewable origin alone does not ensure technical effectiveness or environmental superiority because feedstock characteristics, processing conditions, product purity, and biodegradation behavior strongly influence final performance (Charoentanaworakun et al., 2023; Siwayanan et al., 2021; Tobori et al., 2019; Vega et al., 2025).

Coconut oil represents a promising oleochemical feedstock, particularly in Indonesia and other coconut-producing regions. Its fatty-acid profile is dominated by medium-chain saturated fatty acids, especially lauric and myristic acids. Following transesterification, the resulting FAME mixture can be converted into methyl ester sulfonate (MES), an anionic surfactant whose ester-linked hydrophobic chain and sulfonate headgroup determine solubility, aggregation, interfacial adsorption, and detergency. Previous studies have demonstrated MES production from virgin coconut oil and other renewable lipid feedstocks (Qadariyah et al., 2022; Rawat et al., 2025). However, the influence of coconut-oil variability on FAME reproducibility, sulfonation selectivity, MES composition, application performance, and biodegradation remains insufficiently understood (Amaliah et al., 2021; Pramesti et al., 2026; Qadariyah et al., 2022, 2024; Soy et al., 2020; Syamsuddin et al., 2023).

MES provides several advantages, including renewable carbon content, strong surface activity, detergency at relatively low active concentration, and favorable biodegradation characteristics. Nevertheless, these properties depend strongly on feedstock quality and reaction severity. Moisture, free fatty acids, oxidation products, incomplete transesterification, and fatty-acid distribution can influence FAME quality and subsequent sulfonation behavior. Excessive sulfonation may increase disalt formation, color development, and secondary products, whereas insufficient reaction severity may result in incomplete conversion (Charoentanaworakun et al., 2023; Choptumdee et al., 2021; Maurad et al., 2020; Sailah et al., 2021; Siwayanan et al., 2021).

The optimization of MES synthesis therefore requires balancing multiple responses rather than maximizing a single parameter. Increasing conversion or active matter may appear beneficial; however, excessive reaction severity can reduce interfacial efficiency, biodegradability, and formulation performance. Multiresponse optimization supported by independent validation is therefore necessary to identify robust operating conditions (Rawat et al., 2025; Singh et al., 2022; Yusuff et al., 2023).

Interfacial properties provide important indicators of surfactant behavior, but practical cleaning performance also depends on soil characteristics, water hardness, temperature, and formulation interactions. Therefore, optimized MES should be evaluated using multiple representative soils and compared with established reference surfactants under controlled conditions (Danov et al., 2021; Low et al., 2021; Yavrukova et al., 2020).

Environmental evaluation requires similar consideration. Biodegradation is influenced by molecular structure, chain distribution, product purity, microbial inoculum, and secondary products. Standardized biodegradation procedures require appropriate controls and validity assessment rather than interpretation based solely on the final degradation percentage (OECD, 1992). Preliminary environmental screening provides useful comparative information but does not replace complete ecotoxicological assessment (OECD, 1984, 1992, 2026; Vega et al., 2025).

This study developed an integrated feedstock–process–structure–performance–degradation framework for coconut-oil-derived MES. The objectives were to characterize coconut oil and FAME reproducibility, optimize MES synthesis using a three-factor Box–Behnken design, validate the optimum condition experimentally, compare optimized MES with LAS and SLES references, evaluate detergency and biodegradation performance, and assess its application in liquid-detergent formulations.

Method

Experimental Design and Materials

This study employed an integrated feedstock–process–structure–performance–degradation experimental framework for the production and evaluation of coconut-oil-derived methyl ester sulfonate (MES). The experimental unit was defined as one independent MES synthesis batch, while repeated measurements from the same batch were considered analytical replicates (Qadariyah et al., 2022; Siwayanan et al., 2021).

The experimental workflow consisted of five stages: (1) coconut oil characterization and FAME preparation, (2) MES synthesis optimization, (3) physicochemical and interfacial characterization, (4) detergency and biodegradation evaluation, and (5) liquid-detergent formulation assessment.

Purified coconut oil was used as the renewable feedstock. Methanol and sodium hydroxide were used for FAME preparation through base-catalyzed transesterification. Sulfur trioxide-based sulfonation was performed for MES synthesis, followed by neutralization using sodium hydroxide. Commercial sodium laureth sulfate (SLES) and linear alkylbenzene sulfonate (LAS) were used as reference surfactants (Qadariyah et al., 2022; Soy et al., 2020).

Feedstock Standardization and FAME Production

Coconut oil was characterized for water content, free fatty acid (FFA) content, acid value, peroxide value, saponification value, and fatty-acid composition using standard analytical procedures (Qadariyah et al., 2022; Soy et al., 2020).

The fatty-acid profile was determined by gas chromatography after conversion of fatty acids into their corresponding methyl esters. Particular attention was given to lauric, myristic, palmitic, caprylic, and capric acid fractions because these components determine the molecular characteristics of the resulting MES (Soy et al., 2020; Amaliah et al., 2021).

FAME was produced through base-catalyzed transesterification. Following reaction completion, glycerol was separated, residual alcohol was removed, and the FAME phase was purified before sulfonation (Cohen et al., 2008; Maurad et al., 2020; Nagy et al., 2020; Siwayanan et al., 2021; Yavrukova et al., 2020). FAME conversion was quantified by gas chromatography using an internal standard method.

MES Synthesis and Box–Behnken Optimization

MES synthesis was optimized using a three-factor Box–Behnken experimental design consisting of 17 experimental runs, including five center-point replicates. The investigated factors were: sulfonating-agent-to-FAME molar ratio; reaction temperature; aging time. The factor levels were (Yusuff et al., 2023; Singh et al., 2021; Rawat et al., 2025).

Table 1. Box–Behnken factors and response objectives

Factor	Low	Center	High
Sulfonating-agent/FAME ratio	1.05	1.15	1.25
Temperature (°C)	70	80	90
Aging time (min)	30	60	90

Following sulfonation and aging, products were neutralized and conditioned prior to analysis. The optimization responses included: active MES content; residual FAME; disalt content; color; critical micelle concentration (CMC); minimum surface tension; detergency; biodegradation after 28 days. Multiresponse desirability analysis was applied to maximize active MES, detergency, and biodegradation while minimizing residual FAME, disalt, color, CMC, and surface tension (Maurad et al., 2020; Yusuff et al., 2023).

The chemical structure of MES was confirmed using Fourier-transform infrared spectroscopy (FTIR) (Nurliana et al., 2021). Active MES content, residual FAME, and disalt concentration were determined using validated analytical procedures following previously reported MES characterization approaches (Qadariyah et al., 2022; Maurad et al., 2020).

Surface tension measurements were performed at 25 °C using an IKA tensiometer equipped with a Du Noüy platinum ring. Measurements were conducted at concentrations below and above the expected CMC.

The CMC was determined from the breakpoint of the surface-tension-versus-log-concentration relationship (Danov et al., 2021). The optimized MES was compared with: over-sulfonated MES; LAS reference; SLES reference (Asselah et al., 2017). Additional performance parameters included wetting time, emulsion stability, foam behavior, and rinse performance.

Detergency Evaluation

Detergency performance was evaluated using standardized cotton fabric swatches contaminated with representative soils: synthetic sebum; palm oil; milk-protein soil; carbon–oil mixture. Optimized MES, over-sulfonated MES, LAS, and SLES were tested at equivalent active-surfactant concentrations (Yavrukova et al., 2020; Low et al., 2021; Lynn & Nguyen, 2020).

Washing experiments were conducted under different water-hardness conditions: 50 mg $CaCO_3$/L; 150 mg $CaCO_3$/L; 300 mg $CaCO_3$/L; and temperatures: 20 °C; 40 °C. Stain removal was determined from reflectance changes before and after washing. Soil redeposition was evaluated using clean cotton substrates washed under identical conditions.

This factorial approach was applied to evaluate the interaction between surfactant type, soil composition, hardness level, and washing temperature (Yavrukova et al., 2020; Low et al., 2021; Qadariyah et al., 2024; Choptumdee et al., 2021).

Biodegradation and Environmental Screening

Aerobic biodegradation was evaluated for 28 days using the OECD 301B carbon dioxide evolution method (OECD, 1992). The tested samples included: optimized MES; over-sulfonated MES; LAS; SLES; positive reference compound (OECD, 1992; OECD, 2011).

Biodegradation was calculated from blank-corrected cumulative theoretical CO_2 evolution. Environmental screening was performed through: activated-sludge respiration inhibition; 72-h algal-growth inhibition; seed-germination index evaluation (OECD, 2010; OECD, 2011). These tests were interpreted as comparative environmental screening assessments and were not considered substitutes for complete ecotoxicological risk evaluation (OECD, 2010; OECD, 2011).

Liquid-Detergent Formulation and Stability Evaluation

A liquid-detergent platform containing 12% active surfactant was prepared to evaluate the application potential of optimized MES. Three formulations were evaluated: (Luciana et al., 2022; Yusmin et al., 2025).

All-MES formulation
- 12% active MES

MES/SLES blend
- 8% active MES
- 4% active SLES

All-SLES reference
- 12% active SLES

The formulations contained sodium citrate as builder, sodium carbonate for alkalinity adjustment, and carboxymethyl cellulose as an anti-redeposition and rheology modifier. The formulations were evaluated for: pH; viscosity; foam characteristics; detergency; turbidity; phase stability; active matter retention; color development (Low et al., 2021; Yusmin & Jumal, 2025; Morigaki & Kakizawa, 2021). Storage stability was evaluated at 5, 25, and 40 °C for 12 weeks (Danov et al., 2021; Morigaki & Kakizawa, 2021).

Statistical Analysis

Response surface modeling was performed using quadratic polynomial models. Model adequacy was evaluated through: analysis of variance (ANOVA); lack-of-fit testing; adjusted and predicted R^2 values; residual diagnostics.

The predicted optimum condition was experimentally validated using five independent MES synthesis batches. Detergency data were analyzed using factorial ANOVA considering surfactant type, soil type, water hardness, and temperature as experimental factors. All experimental results were expressed as mean ± standard deviation, and all raw measurements, instrument records, and sample information were maintained for data traceability (Yusuff et al., 2023; Singh et al., 2021; Choptumdee et al., 2021).

Result and Discussion

Feedstock Quality, FAME Reproducibility, and MES Optimization

The quality of the coconut oil feedstock strongly influenced the reproducibility of FAME production and subsequent MES synthesis. The experimental characterization showed that coconut oil contained 0.12% water, 0.19% free fatty acids (expressed as lauric acid), an acid value of approximately 0.41 mg KOH g^{-1}, a low peroxide value, and a saponification value of approximately 256 mg KOH g^{-1}. These characteristics indicated that the feedstock was suitable for base-catalyzed transesterification without intensive acid pretreatment.

The fatty-acid composition was dominated by lauric acid (48.95%), followed by myristic acid (18.13%) and palmitic acid (8.99%), with significant caprylic and capric acid fractions. The combined lauric and myristic acid content reached 67.08%, confirming the dominance of medium-chain C12–C14 fatty acids. This composition is important because the hydrophobic chain length influences MES solubility, aggregation behavior, interfacial adsorption, and interaction with oily contaminants (Qadariyah et al., 2022).

Five independent FAME batches showed conversion above 98%, approximately 0.20% total glycerol, and 0.078% water content. The high reproducibility demonstrated that the transesterification stage provided a consistent substrate for sulfonation. Maintaining FAME quality is essential because residual FAME in the final MES product may originate from incomplete esterification or insufficient sulfonation.

Table 2. Experimental Characteristics of Coconut Oil Feedstock, FAME Substrate, and Optimized MES Product

Metric	Experimental mean	Interpretation
Oil water (%)	0.12	Suitable for base-catalyzed transesterification
Oil FFA (%)	0.19	Low pretreatment requirement
Lauric + myristic (%)	67.08	C12–C14 dominant fatty-acid composition
FAME conversion (%)	98.52	Reproducible FAME substrate
FAME water (%)	0.078	Low hydrolysis risk during sulfonation
Optimum active MES (%)	85.8	Optimum product-quality region achieved
Residual FAME / disalt (%)	5.2 / 5.7	Within established quality targets

The Box–Behnken optimization demonstrated that sulfonating-agent-to-FAME molar ratio, reaction temperature, and aging time significantly affected MES quality. Lower reaction severity resulted in higher residual FAME and reduced active MES formation, indicating incomplete conversion. Increasing reaction severity improved sulfonation efficiency initially; however, excessive temperature, reagent ratio, and aging promoted disalt formation, color development, and secondary reactions.

The response surface analysis identified an internal optimum rather than a boundary condition, demonstrating that maximum reaction intensity did not produce the highest-quality product. The optimum condition was obtained at a sulfonating-agent-to-FAME molar ratio of 1.180, reaction temperature of 81.2 °C, and aging time of 67 min, with an overall desirability value of 0.709 (Figure 1).

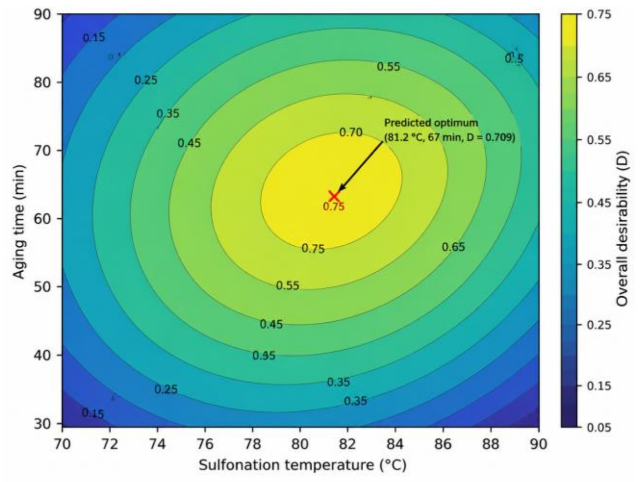

Figure 1. Experimental desirability surface showing the optimum sulfonation region at a molar ratio of 1.180

Five independent experimental validation batches confirmed the predicted optimum, producing 85.8% active MES, 5.2% residual FAME, and 5.7% disalt. These results indicate that process optimization should focus on functional surfactant yield rather than chemical conversion alone. Excessive sulfonation increased non-optimal secondary products without proportional improvement in surfactant performance (Yusuff et al., 2023; Rawat et al., 2025).

Interfacial Properties and Detergency Performance

The optimized MES exhibited favorable interfacial characteristics compared with commercial reference surfactants. The minimum surface tension of optimized MES was 31.40 mN m^{-1}, while the critical micelle concentration (CMC) was 0.75 mM (Table 3). Although LAS produced the lowest surface tension (29.75 mN m^{-1}), optimized MES exhibited efficient micelle formation at a lower concentration than LAS and SLES.

The lower CMC of optimized MES indicates effective molecular organization in aqueous systems. However, interfacial performance is influenced not only by surface tension but also by molecular composition, aggregation behavior, and secondary products. The over-sulfonated MES exhibited higher surface tension (32.24 mN m^{-1}), higher CMC (0.88 mM), longer wetting time, and lower detergency, indicating that excessive sulfonation negatively affected molecular organization.

Table 3. Experimental Comparison of Interfacial Properties and Cleaning-Related Performance Indicators of Optimized MES, Over-sulfonated MES, and Commercial Reference Surfactants

Surfactant	Surface tension (mN/m)	CMC (mM)	Wetting time	Hard-water detergency (%)	Relative rinse volume
LAS reference	29.75	1.19	35.0 s	79.0	4.09
Optimized MES	31.40	0.75	45.5 s	79.4	2.94
Over-sulfonated MES	32.24	0.88	58.0 s	69.6	3.45
SLES reference	30.68	0.93	41.3 s	75.3	3.88

These results confirm that surface tension alone is insufficient for evaluating MES quality. The combination of chemical composition, CMC, adsorption behavior, and detergency response provides a more complete assessment of surfactant performance (Danov et al., 2021).

The detergency evaluation showed that optimized MES performed particularly well toward lipid-based soils. Under hard-water conditions (300 mg $CaCO_3$/L) at 20 °C, optimized MES achieved 77.6% palm-oil removal and 75.4% synthetic-sebum removal, demonstrating effective interaction with hydrophobic soils (Yavrukova et al., 2020; Low et al., 2021; Lynn & Nguyen, 2020).

The favorable lipid-soil removal was associated with the C12–C14 chain distribution derived from coconut oil. Medium-chain hydrophobic groups provide sufficient interaction with oily contaminants while maintaining aqueous dispersion through the sulfonate headgroup (Soy et al., 2020; Siwayanan et al., 2021; Yavrukova et al., 2020; Cohen et al., 2008; Nagy & Theiner, 2020).

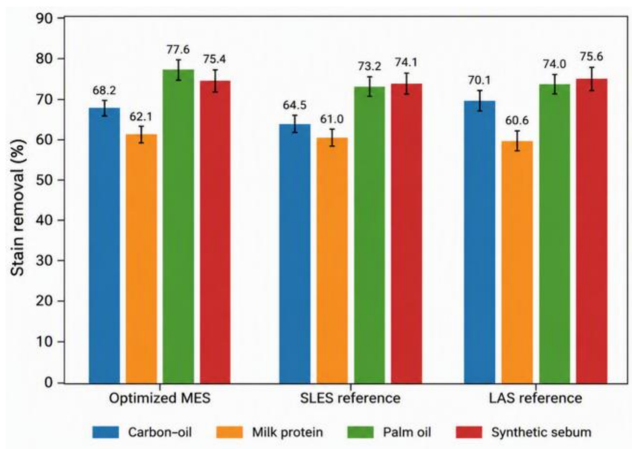

Figure 2. Experimental stain removal under hard-water and low-temperature conditions (300 mg $CaCO_3$/L, 20 °C)

Protein-based soil removal showed a different trend, with SLES maintaining a slight advantage. This difference is attributed to the contribution of wetting, dispersion, and electrostatic interactions in protein removal mechanisms. Carbon–oil soil remained the most difficult substrate because removal required simultaneous oil mobilization and carbon particle suspension (Low et al., 2021; Lynn & Nguyen, 2020).

Water hardness reduced detergency for all surfactants; however, optimized MES maintained competitive performance. These results demonstrate that detergency depends on multiple interactions among surfactant structure, soil characteristics, hardness, and temperature rather than a single surfactant property (Yavrukova et al., 2020; Low et al., 2021; Lim et al., 2019).

Biodegradation and Environmental Screening

The optimized MES demonstrated favorable aerobic biodegradation behavior, exceeding 60% theoretical CO_2 evolution at approximately day 14 and reaching 82.3% biodegradation after 28 days. The positive control achieved 90.7%, while SLES, over-sulfonated MES, and LAS achieved 77.2%, 69.7%, and 65.2%, respectively (Figure 3) (OECD, 1992; Siwayanan et al., 2021; Vega et al., 2025).

The higher biodegradation performance of optimized MES compared with over-sulfonated MES indicates that product composition plays an important role in microbial degradation. Excessive sulfonation increased secondary-product formation, which may reduce microbial accessibility and alter degradation kinetics (Siwayanan et al., 2021; Vega et al., 2025).

The biodegradation results confirm that active MES content alone cannot predict environmental performance. Residual FAME, disalt content, and other reaction products must also be considered. The interpretation followed OECD 301B principles, including consideration of blank validity, positive control performance, and degradation profiles rather than relying only on the final day-28 value (Adiwibowo et al., 2022).

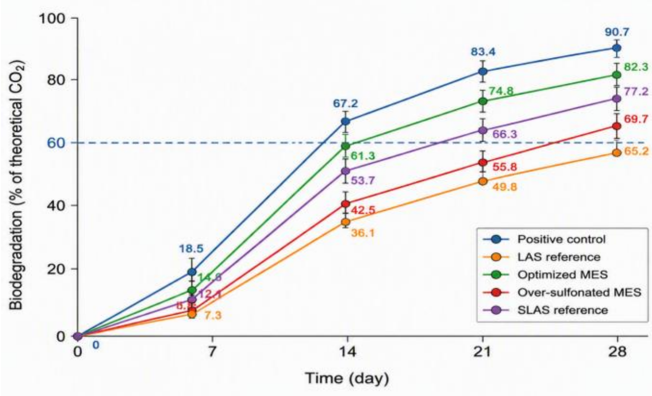

Figure 3. Experimental aerobic biodegradation profiles based on cumulative theoretical CO_2 evolution

Preliminary environmental screening supported the favorable profile of optimized MES. Activated-sludge respiration inhibition was 13.9%, algal-growth inhibition was 17.5%, and the germination index reached 93.4%. These results indicate relatively low inhibitory effects under the tested conditions; however, further concentration–response ecotoxicity studies are required before regulatory conclusions can be established (OECD, 2010; OECD, 2011).

Liquid-Detergent Formulation Performance and Stability

The optimized MES was incorporated into a 12% active liquid-detergent system to evaluate its practical application potential. The all-MES formulation achieved 80.4% detergency, which was comparable with the all-SLES reference formulation (81.2%). The MES/SLES blend achieved the highest detergency (82.5%), suggesting improved interfacial behavior due to combined surfactant interactions (Low et al., 2021; Yusmin & Jumal, 2025; Luciana & Rizkiah, 2022).

The all-MES formulation exhibited a lower viscosity (810 mPa·s) compared with the SLES formulation (1053 mPa·s). Although lower viscosity may facilitate dosing, rheological adjustment may be required to achieve consumer-preferred product characteristics (Lynn & Nguyen, 2020; Low et al., 2021).

Table 4. Experimental Environmental-Screening Responses and Liquid-Detergent Formulation Performance Indicators

Indicator	Optimized MES formulation	Comparator signal
Activated-sludge respiration inhibition (%)	13.9	Lower than LAS (31.8%)
Algal-growth inhibition (72 h) (%)	17.5	Lower than LAS (40.3%)
Germination index (%)	93.4	Above 90% screening level
Formulation detergency (%)	80.4	SLES formulation: 81.2%
Formulation viscosity (mPa·s)	810	SLES formulation: 1053 mPa·s
Active matter after storage at 40 °C for 12 weeks (%)	11.89	Slight decrease from initial value

During the 12-week storage study, all formulations maintained acceptable stability at 25 °C without major phase separation. At 40 °C, MES-containing formulations showed slight color development and minor active-matter reduction. The all-MES formulation retained 11.89% active matter after 12 weeks at 40 °C (Low et al., 2021; Yusmin & Jumal, 2025).

The saturated C12–C14 homolog distribution may contribute to low-temperature solubility challenges due to Krafft-phase behavior. Therefore, future development should include freeze–thaw evaluation, low-temperature microscopy, packaging compatibility testing, and long-term stability assessment (Danov et al., 2021; Morigaki & Kakizawa, 2021).

Mechanistic Interpretation and Scale-Up Implications

The experimental findings demonstrate a continuous relationship between feedstock composition, sulfonation conditions, MES molecular structure, interfacial behavior, cleaning performance, and biodegradation (Siwayanan et al., 2021; Yusuff et al., 2023; Rawat et al., 2025).

The C12–C14 fatty-acid distribution of coconut oil influenced hydrophobicity and aqueous compatibility, while sulfonation conditions controlled the balance between desired MES formation and secondary-product generation. At the molecular level, active MES concentration and homolog distribution affected CMC and adsorption behavior, whereas residual FAME and disalt influenced interfacial efficiency and biodegradation (Soy et al., 2020; Maurad et al., 2020; Nurliana et al., 2021).

At the application level, detergent performance emerged from interactions among surfactant composition, soil characteristics, water hardness, temperature, and formulation components. These findings explain why excessive reaction severity did not correspond to maximum product performance (Yavrukova et al., 2020; Low et al., 2021; Asselah et al., 2017).

The optimized process therefore represents a balanced operating region where chemical quality, application performance, and environmental compatibility are simultaneously achieved (Yusuff et al., 2023; Rawat et al., 2025; Choptumdee et al., 2021).

Conclusion

This study demonstrated that coconut-oil-derived methyl ester sulfonate (MES) can be successfully developed as a renewable anionic surfactant through an integrated feedstock–process–structure–performance–degradation framework. The C12–C14-rich fatty-acid composition of coconut oil provided a suitable precursor for FAME production, while Box–Behnken optimization identified the optimum sulfonation condition at a sulfonating-agent-to-FAME molar ratio of 1.180, a reaction temperature of 81.2 °C, and an aging time of 67 min. Experimental validation confirmed the production of MES with 85.8% active matter, 5.2% residual FAME, 5.7% disalt, favorable interfacial properties, 77.2% detergency, and 82.3% biodegradation after 28 days. Excessive sulfonation reduced overall product quality by increasing secondary-product formation and decreasing interfacial efficiency and biodegradation performance. The optimized MES showed competitive performance compared with commercial LAS and SLES references and was successfully incorporated into a 12% active liquid-detergent formulation. The all-MES formulation achieved comparable detergency to the SLES reference, while the MES/SLES blend provided additional performance improvement. Overall, the results demonstrate that balanced sulfonation optimization, rather than maximum reaction severity, is essential for achieving MES with desirable chemical quality, cleaning performance, and biodegradability. Further pilot-scale validation, detailed ecotoxicological assessment, life-cycle analysis, and techno-economic evaluation are required before industrial implementation.

Acknowledgments

The authors sincerely acknowledge the Faculty of Mathematics and Natural Sciences, University of Tadulako, for providing laboratory facilities and institutional support during this research. The authors also thank colleagues and laboratory members who contributed to experimental activities, analytical measurements, and data evaluation.

Author Contributions

Conceptualization, Syamsuddin and Jusman; methodology, Syamsuddin; software, Syamsuddin; validation, Syamsuddin and Jusman; formal analysis, Syamsuddin; investigation, Syamsuddin; resources, Jusman; data curation, Syamsuddin; writing—original draft preparation, Syamsuddin; writing—review and editing, Syamsuddin and Jusman; visualization, Syamsuddin; supervision, Jusman; project administration, Jusman; funding acquisition, Jusman. All authors have read and agreed to the published version of the manuscript.

Funding

This research was funded independently by the authors.

Conflicts of Interest

The authors declare no conflict of interest.

References

Adiwibowo, M. T., Sukarya, A., Putra, F. R. A., Pramudita, M., Hartono, R., & Pitaloka, A. B. (2022). Degradation of methyl ester sulfonate using TiO2 photocatalyst. *Teknika: Jurnal Sains Dan Teknologi*, *18*(2), 119. https://doi.org/10.36055/tjst.v18i2.16940

Amaliah, D., Qadariyah, L., & Mahfud, M. (2021). The Production of Surfactant Anionic Methyl Ester Sulfonate (MES) from Virgin Coconut Oil (VCO) with Ultrasound-Assisted. *Journal of Physics: Conference Series*, *1845*(1), 012005. https://doi.org/10.1088/1742-6596/1845/1/012005

Asselah, A., Pinazo, A., Mezei, A., Pérez, L., & Tazerouti, A. (2017). Self-Aggregation and Emulsifying Properties of Methyl Ester Sulfonate Surfactants. *Journal of Surfactants and Detergents*, *20*(6), 1453–1465. https://doi.org/10.1007/s11743-017-2026-9

Charoentanaworakun, C., Assabumrungrat, S., & Soottitantawat, A. (2023). Techno-Economic-Environmental Analysis of Sustainable Anionic Biosurfactant Production from Palm Fatty Acid Distillate. *ACS Omega*, *8*(47), 45045–45055. https://doi.org/10.1021/acsomega.3c06777

Choptumdee, K., Kittisupakorn, P., & Daosud, W. (2021). Heat Integration Design of Alpha Methyl Ester Sulfonate Production Process. *Process Integration and Optimization for Sustainability*, *5*(4), 745–754. https://doi.org/10.1007/s41660-021-00186-3

Cohen, L., Soto, F., Melgarejo, A., & Roberts, D. W. (2008). Performance of Φ-Sulfo Fatty Methyl Ester Sulfonate Versus Linear Alkylbenzene Sulfonate, Secondary Alkane Sulfonate and α-Sulfo Fatty Methyl Ester Sulfonate. *Journal of Surfactants and Detergents*, *11*(3), 181–186. https://doi.org/10.1007/s11743-008-1069-3

Danov, K. D., Stanimirova, R. D., Kralchevsky, P. A., Slavova, T. G., Yavrukova, V. I., Ung, Y. W., Tan, E., Xu, H., & Petkov, J. T. (2021). Solubility of ionic surfactants below their Krafft point in mixed micellar solutions: Phase diagrams for methyl ester sulfonates and nonionic cosurfactants. *Journal of Colloid and Interface Science*, *601*, 474–485. https://doi.org/10.1016/j.jcis.2021.05.147

Low, S. Y., Tan, J. Y., Ban, Z. H., & Siwayanan, P. (2021). Performance of Green Surfactants in the Formulation of Heavy-Duty Laundry Liquid Detergents (HDLD) with Special Emphasis on Palm Based Alpha Methyl Ester Sulfonates (α-MES). *Journal of Oleo Science*, *70*(8), ess21078. https://doi.org/10.5650/jos.ess21078

Luciana, L., & Rizkiah, R. (2022). Utilization Of Methyl Ester Sulfonate As a Surfactant Raw Material in the Scouring, Bleaching and Dyeing Process of Rayon Fabric. *Technium Sustainability*, *2*(2), 23–31. https://doi.org/10.47577/sustainability.v2i2.6079

Lynn, J. L., & Nguyen, T. (2020). Detergents and Detergency. In *Bailey's Industrial Oil and Fat Products* (pp. 1–46). Wiley. https://doi.org/10.1002/047167849X.bio033.pub2

Maurad, Z. A., Abdullah, L. C., Anuar, M. S., Shah, N. N. A. K., & Idris, Z. (2020). Preparation, Characterization, Morphological and Particle Properties of Crystallized Palm-Based Methyl Ester Sulphonates (MES) Powder. *Molecules*, *25*(11), 2629. https://doi.org/10.3390/molecules25112629

Nagy, A., & Theiner, E. (2020). Detergency and Detergents. In *Kirk-Othmer Encyclopedia of Chemical Technology* (pp. 1–64). Wiley. https://doi.org/10.1002/0471238961.0405200512251414.a01.pub3

Nurliana, L., Kadidae, L. O., Sunarti, S., & Musta, R. (2021). Characterization of Methyl Ester Sulfonate (MES) from Mahagony (Swietenia macrophylla King) with Variations in H2SO4 Concentration and Sulfonation Duration. *ALCHEMY Jurnal Penelitian Kimia*, *17*(2), 192. https://doi.org/10.20961/alchemy.17.2.51613.192-201

OECD. (1984). *Test No. 209: Activated Sludge, Respiration Inhibition Test*. OECD Publishing. https://doi.org/10.1787/9789264070080-en

OECD. (1992). *Test No. 301: Ready Biodegradability*. OECD. https://doi.org/10.1787/9789264070349-en

OECD. (2026). *Test No 201 Alga Growth Inhibition Test*. OECD Publishing. https://doi.org/10.1787/9789264069923-en

Pramesti, I. N., Iqbal, M. A., Retnosari, R., & Octaviana, L. (2026). Ultrasonic-Assisted Synthesis of Methyl Ester Sulfonate (MES) from Coconut Oil via Transesterification and Sulfonation Using Eggshell-Derived CaO Catalyst. *Al-Kimia*, *14*(1). https://doi.org/10.24252/al-kimia.v14i1.62602

Qadariyah, L., Ryvalda, D. S., Aditama, N. Y., Aswie, V., & Mahfud, M. (2024). Methyl Ester Sulfonate (MES) Surfactant Production from Waste Cooking Oil (WCO) with Microwave Technology. *Science and Technology Indonesia*, *9*(4), 929–940. https://doi.org/10.26554/sti.2024.9.4.929-940

Qadariyah, L., Sahila, S., Sirait, C., Purba, C. P. E., Bhuana, D. S., & Mahfud, M. (2022). Surfactant Production of Methyl Ester Sulfonate from Virgin Coconut Oil using Aluminum Oxide with Microwave Assistance. *International Journal of Technology*, *13*(2), 378. https://doi.org/10.14716/ijtech.v13i2.4449

Rawat, N., Alam, P., Bhonsle, A. K., Ngomade, S. B. L., Agarwal, T., Singh, R. K., & Atray, N. (2025). Valorization of used cooking oil into bio-based surfactant: modeling and optimization using response surface methodology. *Biomass Conversion and Biorefinery*, *15*(17), 24243–24257. https://doi.org/10.1007/s13399-024-05753-5

Sailah, I., Hambali, E., & Aulyana, F. E. (2021). Formulation of Biodegreaser Made from Palm Oil Methyl Ester Sulfonate Surfactant with Oxalic Acid

Additive. *International Journal of Oil Palm*, *4*(2), 39–45. https://doi.org/10.35876/ijop.v4i2.62

Singh, N., Gupta, S. K., & Yadav, P. K. S. (2022). RSM-Based Optimization Approach in Production of Anionic Methyl Ester Sulfonate for Commercial Detergent Application. *Journal of The Institution of Engineers (India): Series E*, *103*(2), 283–291. https://doi.org/10.1007/s40034-021-00234-0

Siwayanan, P., Ban, Z. H., Zhang, X., & Parthiban, A. (2021). <scp>α-Sulfo</scp> Fatty Methyl Ester Sulfonate: A Review on Chemistry, Processing Technologies, Performance, and Applications in Laundry Detergents. *Journal of Surfactants and Detergents*, *24*(3), 385–399. https://doi.org/10.1002/jsde.12509

Soy, R. C., Kipkemboi, P. K., & Rop, K. (2020). Synthesis, Characterization, and Evaluation of Solution Properties of Sesame Fatty Methyl Ester Sulfonate Surfactant. *ACS Omega*, *5*(44), 28643–28655. https://doi.org/10.1021/acsomega.0c03698

Syamsuddin, S., & Jusman, J. (2023). Formation of Methyl Ester Sulfonate (MES) from Pure Coconut Oil Material as Surfactant. *International Journal of Research Publication and Reviews*, *4*(10), 3408–3410. https://doi.org/10.55248/gengpi.4.1023.102907

Tobori, N., & Kakui, T. (2019). Methyl Ester Sulfonate. In *Biobased Surfactants* (2nd ed., pp. 303–324). Elsevier. https://doi.org/10.1016/B978-0-12-812705-6.00009-5

Vega, G. R., & Stampino, P. G. (2025). Bio-Based Surfactants and Biosurfactants: An Overview and Main Characteristics. *Molecules*, *30*(4), 863. https://doi.org/10.3390/molecules30040863

Yavrukova, V. I., Shandurkov, D. N., Marinova, K. G., Kralchevsky, P. A., Ung, Y. W., & Petkov, J. T. (2020). Cleaning Ability of Mixed Solutions of Sulfonated Fatty Acid Methyl Esters. *Journal of Surfactants and Detergents*, *23*(3), 617–627. https://doi.org/10.1002/jsde.12393

Yusmin, I., & Jumal, J. (2025). Synthesis and characterization of methyl ester sulfonate surfactant based on used cooking oil as an active ingredient in laundry liquid detergent. *Malaysian Journal of Analytical Sciences*, *29*(1). Retrieved from https://mjas.analis.com.my/mjas/v29_n1/html/29_1_1185.html

Yusuff, A. S., Ishola, N. B., & Gbadamosi, A. O. (2023). Artificial Intelligence Techniques and Response Surface Methodology for the Optimization of Methyl Ester Sulfonate Synthesis from Used Cooking Oil by Sulfonation. *ACS Omega*, *8*(22), 19287–19301. https://doi.org/10.1021/acsomega.2c08117