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Simulating the Production of Surfactant α-MES (a Methyl Ester Sulfonate) from FAME (Fatty Acid Methyl Ester) Using the Superpro Designer Application

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ABSTRACT

The demand for energy continues to grow, while the availability of fossil fuel-based energy is gradually decreasing. As the population increases, so does the need for oleochemical products. One commonly utilized product in the oleochemical industry is surfactants. These are molecules characterized by the presence of both hydrophilic (water-attracting) and lipophilic (oil-attracting) groups in a single structure. The production of surfactants from FAME (Fatty Acid Methyl Ester) begins with a sulfonation step, during which FAME reacts with a reagent like oleum SO_3. However, to ensure the process is efficient and effective, optimization is necessary. A detailed simulation using SuperPro Designer software can help model the production process. The results of these simulations reveal that optimizing parameters such as temperature, pressure, and reactant ratios can significantly enhance the production efficiency of surfactants. Therefore, process optimization through simulation can be a key factor in improving both the efficiency and sustainability of the oleochemical industry.

1. Introduction

Currently, biodiesel, green gasoline, and biosyngas are among the most favored alternative fuels worldwide. The growing focus on renewable energy research and development stems from the numerous advantages bioenergy offers compared to fossil fuels (Fahmi et al., 2022). For example, biodiesel combustion produces cleaner emissions, significantly reducing carbon monoxide, hydrocarbons, particulate matter, and polyaromatic hydrocarbons, although nitrogen oxide emissions remain relatively high. Despite this limitation, biodiesel is considered an eco-friendly solution. It can be synthesized from various plants, including palm oil, jatropha, coconut oil, soybean oil, and sunflower seeds. In

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Indonesia, palm oil is predominantly used to produce Fatty Acid Methyl Ester (FAME), a key component of biodiesel (Dimawarnita & Hambali, 2021).

The increasing global population drives a rising demand for oleochemical products, particularly surfactants (Putri & Jaya, 2020). Surfactants (surface active agents) are unique molecules that combine hydrophilic (water-attracting) and lipophilic (oil-attracting) groups in their structure. Producing Methyl Ester Sulfonate (MES), a surfactant derived from FAME, begins with the sulfonation process, where FAME reacts with oleum SO3. The choice of reagents and process parameters, such as raw material availability, operational conditions, and economic viability, plays a crucial role in optimizing production. Proper reagent selection ensures the production of high-quality, cost-effective products through an environmentally sustainable process, minimizing waste (Putri & Mustain, 2020).

MES production involves esterification followed by sulfonation, which adds sulfate groups to organic compounds (Putri & Adi, 2016). Critical factors for achieving optimal MES quality include the molar ratio of reactants, reaction temperature and duration, sulfate concentration, sulfonation materials, and conditions for neutralization, such as pH and temperature (Rahmawati, 2021). Studies indicate that the best results for sulfonation depend on specific molar ratios, as the process yields derivatives formed through reactions between sulfate groups and oils, fatty acids, or alcohols (Iman et al., 2016).

This research evaluates the potential for large-scale biodiesel production from FAME using simulations conducted in SuperPro Designer, a chemical process simulator. The study focuses on the transesterification method, which converts triglycerides in vegetable oils into FAME that reacts with SO3 to form surfactants. This method is preferred for its high conversion efficiency, reaching up to 98%. The simulation incorporates key variables, including process efficiency, energy consumption, and raw material usage. The data gathered is then used to develop an economic model, estimating investment and operational costs and assessing profitability. Additionally, the study compares the selling price of the resulting surfactants with other brands in Indonesia to determine their economic feasibility.

2. Research Method

This study examines the potential of FAME (Fatty Acid Methyl Ester) as a raw material for surfactant production, utilizing SuperPro Designer software. The process incorporates sulfonation and esterification methods in the simulation, replacing laboratory experiments and mathematical computations. The research methodology consists of problem identification, literature review, data collection and analysis, and simulation using SuperPro Designer. Once the simulation is completed, the results are validated, and an analysis of the biodiesel production costs is carried out. The steps involved in the research include identifying the problem, reviewing the literature, collecting and processing data, running simulations with SuperPro Designer, validating the simulation outcomes, and conducting a cost analysis of production, As shown in Figure 1, the research steps.

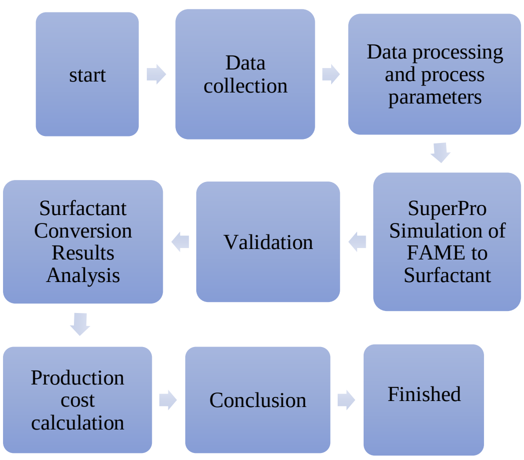

Figure 1. The research steps.

2.1. Data collection

The data for FAME (Fatty Acid Methyl Ester) and other materials like Na_2SO_4, SO_3, CH_3OH, NaOH, H_2O_2, Na_2CO_3 are sourced from various providers. These data can be accessed through the National Standardization Agency (BSN) or the Central Statistics Agency (BPS), which offer detailed information on the quality and specifications of FAME and additional materials, as shown in Tables 1,2, and 3. As for the FAME data in Indonesia, it amounted to 1.701.000 tons in 2022.

Table 1. Data of Raw Material Components for Surfactant Production

No	Component	Rumus Kimia	Chemical formula (g/mol)	Density (g/cm^3)
1.	Metil Laurat	$C_{11}H_{23}COO$	214,34	0.87
2.	Metil Palmitat	$C_{15}H_{31}COOCH_3$	270,5	0,852
3.	Metil Stearat	$C_{17}H_{35}COOCH_3$	298,5	0,845
4.	Metil Miristat	$C_{13}H_{27}COOCH_3$	242,4	0,867
5.	Methanol	CH_3OH	32,04	0,7928
6.	Sodium Hydroxide	NaOH	39,9971	2,13
7.	Hydrogen Peroxide	H_2O_2	34,016	1,11
8.	Natrium Carbonate	Na_2CO_3	105,9888	2,54
9.	Sodium Sulfate	Na_2SO_4	142,04	2,66
10.	Air	O_2	31,999	0,001225
11.	Sulfur Trioxide	SO_3	80,06	1,92

Sources: (Probowati, Giovanni, & Ikhsan, 2012)

Table 2. Data on Production Cost Parameters of Raw Materials

No.	Variable	Cost (Rp)
1.	FAME	10.000
2.	Conversion Cost	14.000
3.	Chemical Price	2.000
4.	Overhead Costs	12.000

Table 3. List of Surfactant Selling Prices

No.	Name	Cost (Rp)
1.	SLES Texapon Emal 270N	123.000
2.	Anionic Flocculant	45.000
3.	Surfaktan α -MES *(α Methyl Ester Sulfonate)*	14.000

2.2. Calculation of a-MES Surfactant (a Methyl Ester Sulfonate) Potential

The conversion of FAME (Fatty Acid Methyl Ester) to MES Surfactant requires processing and calculating raw material data during the mixing of raw materials and reagents to achieve the final product, Surfactant. This simulation uses a modified sulfonation and esterification method, with the help of SuperPro Designer software as a process simulator, carried out in several steps, as follows:

2.2.1 Calculation of the Average Amount of FAME (Fatty Acid Methyl Ester) in Indonesia

To calculate the average monthly amount of FAME produced throughout Indonesia, mathematical calculations are performed using the following formula:

$$m = \frac{Amount\ Data}{Lots\ of\ Data} \qquad \textbf{(2.1)}$$

m = Average amount

2.2.2. Calculation of the Composition of Raw Material Mixing for Surfactant Production

To produce surfactant from FAME, the sulfonation and esterification methods are used, simulated with the Superpro Designer software. This conversion process involves the reaction of FAME with SO_3 to produce MES surfactant. The composition of the raw material mixture is determined based on the research, where the requirement for SO_3 dissolved in air amounts to 60% (inert) of the total FAME raw material, which is mathematically calculated using a specific formula :

$$SO_3\ amount = \frac{60}{100} \times Amount\ of\ FAME \qquad \textbf{(2.2)}$$

$$\text{Surfactant Conversion} = \text{Raw Material FAME} + \text{Amount of } SO_3 \qquad \textbf{(2.3)}$$

2.3. Process Parameters for Superpro Simulation of FAME Surfactant Conversion

Once the raw material composition for converting FAME (Fatty Acid Methyl Ester) into MES surfactant is determined, the process of initiating the simulation using SuperPro Designer can begin (Smith & Jones, 2022).

2.3.1. Flowchart for FAME Surfactant Production using SuperPro Designer Software

Once the raw material composition for converting FAME (Fatty Acid Methyl Ester) into MES surfactant is determined, the steps to initiate the simulation using SuperPro can be followed as outlined in Table 4.

Table 4. Process Parameters for SuperPro Simulation

No	Steps	Description
1.	Process Model Selection	The process mode implemented is the batch method, which enables the adjustment of process scheduling without interrupting other ongoing production processes.
2.	Component Assembly	At this stage, the required components and their related components to be processed in SuperPro Designer are entered.
3.	Process Treatment	In this stage, the type of reactor to be used is chosen, and the supporting components for the selected reactor in the Transesterification and processing steps are entered.
4.	Executing the Simulation	Execute the simulation based on the completed steps to achieve the desired results..

2.3.2.Simulation Process of FAME Conversion into Surfactant Using SuperPro Designer Software

In this process, FAME (Fatty Acid Methyl Ester) and SO_3 are prepared, and process units for converting FAME into MES surfactant are selected in SuperPro Designer, including Mixing, Stirred Reactor, and Hammer Crusher. The Mixing unit combines raw materials, the Reactor unit carries out the esterification reaction of FAME and methanol, followed by crushing to ensure uniformity and mixing with Na_2CO_3 to strengthen the surfactant structure. The result is MES surfactant, as shown in Table 5.

Table 5. Surfactant Conversion Simulation Process in SuperPro

No	Unit Procedure	Process
1.	Raw Material Mixing Process in Mixing	Mixing Fatty Acid Methyl Ester with Na_2SO_4. Na_2SO_4 is added as an inhibitor to prevent color change, ensuring that the Methyl Sulfonic Acid (MSA) formed after sulfonation does not turn too dark. Additionally, in the preparation stage, SO_3 is diluted with air
2.	Sulfonation Process in Stirred Reactor	FAME reacts with SO_3 to create SO_3 monoadduct with a 98% conversion. The monoadduct then reacts with additional SO_3 to form SO_3 diadduct with complete conversion. Lastly, the SO_3 diadduct is converted into Methyl Sulfonic Acid (MSA) with an 80% conversion rate.
3.	Esterification Process in Esterification Tank	The production of α-Methyl Ester Sulfonate involves combining the reactor output with a methanol solution in the Esterification Tank. This process is conducted at 80°C and 1 atm pressure for 30 minutes.
4.	Neutralization Process in Neutralization Tank	The reaction between Methyl Sulfonic Acid (MSA) and NaOH produces α-Methyl Ester Sulfonate (α-MES) and water. This process is carried out at 70°C for 20 minutes.

5.	Bleaching Process in Esterification Tank	The production of α-Methyl Ester Sulfonate includes bleaching the α-MES product by combining it with H_2O_2. The bleaching process is conducted at 80°C and 1 atm pressure for 3 hours.
6.	Aging Process in Aging Tank	In this process, the product is mixed in the Aging Tank with a stirrer at 80°C and 1 atm pressure for 3 hours.
7.	Evaporation and Cooling Process in Vacuum Evaporator and Cooling Belt	In this process, the slurry product is evaporated to remove water and methanol, producing a concentrated paste. The evaporation occurs in a Vacuum Evaporator at 120°C and 0.01 atm pressure. Afterward, the product is cooled using a Cooling Belt Conveyor with air flow, with the final product temperature expected to be around 30°C.
8.	Crushing and Mixing Process in Hammer Crusher	In this process, the product from the previous stage (evaporation and cooling) is crushed with a Hammer Crusher to achieve uniform-sized α-MES. The crushed product is then combined with Na_2CO_3 to enhance the structure of the α-Methyl Ester Sulfonate surfactant.

2.4. Simulation Result Verification

The verification conducted in this study involves comparing the results with previous research that has outcomes closely matching the characteristics of the surfactant. This comparison is assisted by SuperPro Designer software and is shown in Table 6.

Table 6. Simulation Result Verification

No	Parameter	Journal	Simulation Results
1.	Raw Material	FAME	FAME
2.	Input Volume (ml)	500	500
3.	Produced Surfactant (ml)	350	382
	Error		9%

According to Table 6, which refers to a study with an input volume of 500 ml of fatty acid methyl ester, the resulting surfactant is 350 ml, while the SuperPro Designer simulation yields 382 ml. The validation shows an error of 9%. Since the error is below 10%, the study is considered valid. This is because the study serves as a reference to verify the simulation results with actual experiments, where external factors like temperature and chemical reactions can affect the outcomes, whereas simulations are not influenced by such factors.

2.5. Surfactant Production Cost Calculation

The aim of this study is to determine the production price index of surfactants made from FAME as the raw material. This calculation is based on a study conducted by Suwarno (Suwarno, 2021), which includes several variables such as raw material costs, conversion costs, chemical prices, and other additional expenses. The formula for calculating the Production Price Index (HIP) is:

HIP = raw material cost + conversion cost **(2.4)**

3. Result and Discussion

3.1.Calculation of the Average Surfactant Production in Indonesia

Using FAME data from Indonesia over the last three years and data from 2022, the monthly average is determined by applying equation (2.1), as shown below:

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$$Average\ FAME = \frac{1.701.000\ (ton)}{12\ month}$$

$$= 141.750 \text{ Ton/month}$$

The calculation results in the average amount of surfactant produced in Indonesia each month.

3.2.Raw Material Mixing Composition Calculation

To produce surfactants, it is necessary to calculate the composition of raw materials for the conversion process, which in this case consists of FAME + SO_3, with the following calculation for a monthly time frame:

a. FAME amount = 141,750 Tons/Month
b. SO3 is dissolved in air at 60% (inert). (US Patent 7,592,3 B2) SO3 amount = 60/100 x 141,750 Tons = 85,000 Tons

Based on the above calculation, to simulate surfactant processing for one month with 141,750 Tons of FAME, 85,000 Tons of SO_3 is required as an additional raw material.

3.3 Surfactant Synthesis Simulation Results Using SuperPro

In the simulation, FAME (Fatty Acid Methyl Ester) and SO_3 undergo a sulfonation process in reactor (R-01) for 1 hour at 80°C and 1 atm pressure. Since the Internal Rate of Return (IRR) is not directly provided in the economic analysis, it is manually calculated using Microsoft Excel, yielding an IRR of 0.41. This indicates that the project is expected to generate an annual return rate of 41%. In other words, the project could provide an average annual profit of 41% As stated in the research by Ardiansyah (Ardiansyah & Pringgo, 2019). Thus, the manual IRR calculation shows that the project has strong profit potential, although careful interpretation and additional analysis are still necessary, As shown in Table 7. Meanwhile The process of surfactant synthesis using SuperPro Designer is illustrated in Figure 2.

Table 7. SuperPro Designer Simulation Result

No.	Parameter	Surfaktan
1.	Flowrate(Kg)	97.738,879
2.	Mass Comp (%)	100
3.	Concentration Kg/m^3	80
4.	Mass Flow(Kg)	253.125
5.	Volumetric Flow(L)	97.485,754
6.	Temperature (^{o}C)	29,73

According to the table above, it is evident that Indonesia can produce 97,485,754 liters of surfactant per month with a mass composition of 100% and a concentration or density of 80 kg/m³.

3.4. Production Cost Analysis for FAME (Fatty Acid Methyl Ester) Surfactant

The production cost of surfactant from FAME (Fatty Acid Methyl Ester) can be determined through mathematical calculations as follows:

1. Average price of FAME: Rp 10,000/liter
2. Conversion cost: Rp 14,000/liter
3. Chemical cost: Rp 2,000
4. Overhead cost: Rp 12,000/liter

Total HIP = (Raw material price + Conversion cost)

a. Conversion cost = (Chemical cost + Overhead cost)
b. Total conversion cost = Rp (2,000 + 12,000)= Rp 14,000
c. Total HIP = Rp (10,000 + 14,000)= Rp 24,000

3.5. Analysis of the Comparison of Selling Prices for Diesel Fuel Products

Referring to the data in Table 5, the selling prices of anionic surfactants from various popular brands in Indonesia vary. For instance, Coco Glucoside can cost approximately Rp 123,000 per liter, while other anionic surfactants range from Rp 15,000 to Rp 127,700 per liter, depending on the brand and type.

When compared to the conversion cost from the SuperPro Designer simulation, which is Rp 14,000 per liter, this price is very competitive and below the average market price. This shows that the price is economically favorable when compared to several other products available in the market.

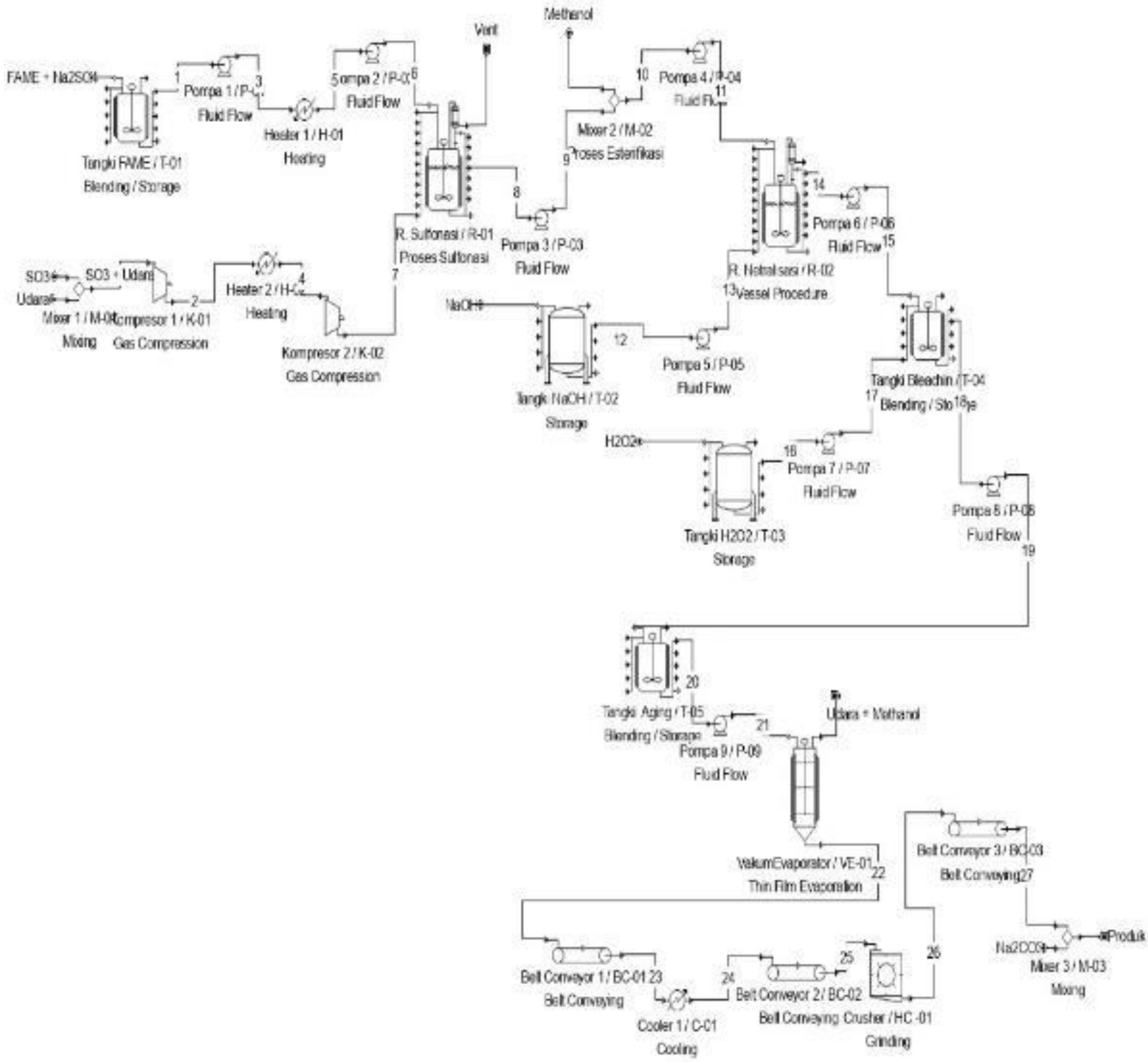

Figure 2. Surfactant Synthesis Process Using SuperPro Designer

4. Conclusion

Based on the results, it can be concluded that 141,750 tons of surfactant per month, when processed using the sulfonation method and assisted by the SuperPro Designer application for simulation, will yield a surfactant with a volumetric flow of 97,485.754 L. The surfactant has a density of 80 Kg/m³. The Production Index Price (HIP) for converting FAME into surfactant is Rp 4,000 per liter. The selling price offered is Rp 14,000 per liter, according to a study by the Ministry of Energy and Mineral Resources (ESDM). This presents a competitive and cost-effective alternative, well below the average market price. This indicates that the price is more economical when compared to other products available in the market.

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Units and Abbreviations

g/mol= gram per mol, g/cm^3= gram per centimeter cubic, Rp= Rupiah, kg= kilogram, g= gram, L= liter, ^{o}C = degrees Celsius, Kg/m3= kilogram per meter cubic, % = Percentage.

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