Nature of Invention: Process design

Applicant: ChemEverse

Inventors: Armaan Pratik Pasayat, Pratyush Biswal

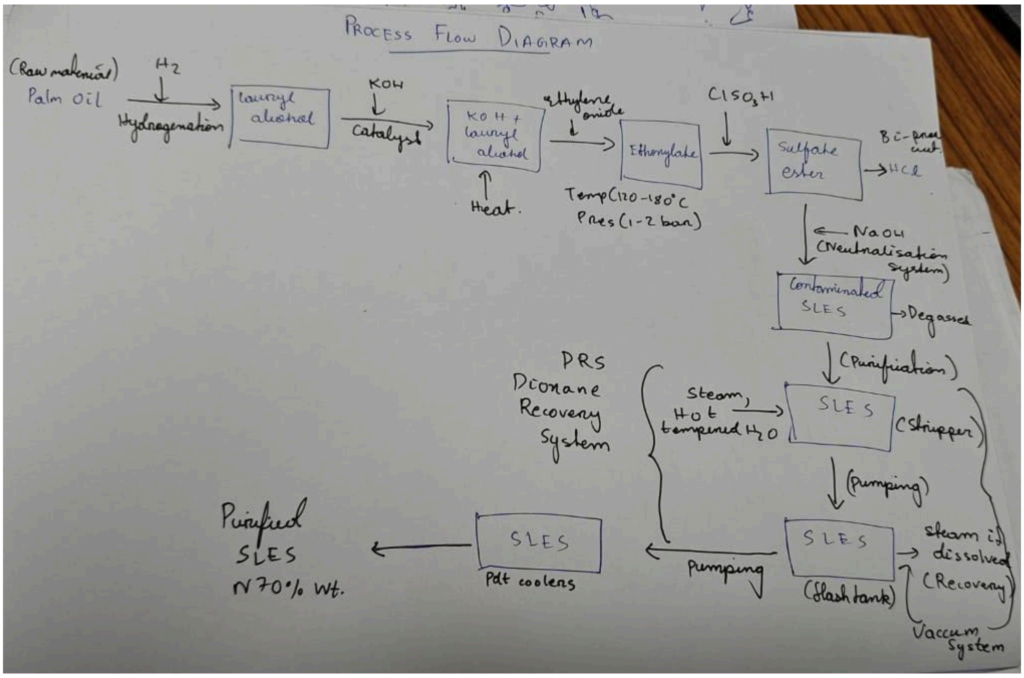
Chemical Formula: $C_{12}H_{25}NaO_4S$

Chemical Name: Sodium Laureth 2-Sulfate (SLES)

Process Title: Production of Sodium Laureth 2-Sulfate (SLES) from Lauryl Alcohol

Process Description:

a. Give the block diagram for the feasible process (as determined in the market analysis report). List all unit operations and process conditions.



b. Give the material balance for a scaled-up process plant with capacity of 1000 kg/day. (If needed, simplify the calculations by stating assumptions)

Mass Balance for SLES - @ 1000 kg/day capacity

Step 1: Hydrogenation of Palm Oil to Lauryl Alcohol

Reaction:

Palm Oil + H_2 ⟶ Lauryl Alcohol.

Input Streams:

- Palm Oil : 1200 kg/day
- Hydrogen Gas (H_2) : 30 kg/day
- Catalyst (KOH) : 5 kg/day

Output Streams:

- Lauryl Alcohol : 980 kg/day
- Glycerin & Light Byproducts : 180 kg/day
- Unreacted Hydrogen & Losses : 75 kg/day

Step 2: Ethoxylation of Lauryl Alcohol

Reaction:

$$C_{12}H_{26}O + n(C_2H_4O) \rightarrow C_{12}H_{26}(OCH_2CH_2)_nOH$$

Input Streams:

- Lauryl Alcohol : 980 kg/day
- Ethylene Oxide (EO) : 490 kg/day
- Catalyst : 2 kg/day

Output Streams:

- Lauryl Ether Alcohol : 1440 kg/day
- Unreacted EO & Losses : 32 kg/day

…3 : Sulfation of Lauryl Ether Alcohol-

Reaction:

$C_{12}H_{26}(OCH_2CH_2)_3OH + SO_3 \rightarrow C_{12}H_{26}(OCH_2CH_2)_3OSO_3H$

Input Streams:

- Lauryl Ether Alcohol : 1440 Kg/day
- SO_3 gas : 360 kg/day
- Solvent Medium : 50 kg/day

Output Streams:

- Sulfated Product (SLES Acid Form): 1740 kg/day
- Unreacted SO_3 & Minor losses: 110 kg/day

Step-4 : Neutralisation with NaOH -

Reaction:

$C_{12}H_{26}(OCH_2CH_2)_3OSO_3H + NaOH \rightarrow C_{12}H_{26}(OCH_2CH_2)_3OSO_3Na + H_2O$

Input streams:

- Sulfated Product : 1740 Kg/day
- NaOH solution (30% w/w) : 150 Kg/day

Output Streams:

- Crude SLES : 1860 Kg/day
- Water Byproduct : 90 Kg/day

-5: Purification & Recovery
(Purification through vacuum stripping, filtration and cooling)

Input Streams -

- Crude SLES : 1860 kg/day
- Water & Processing Additives : 300 kg/day

Output Streams :

- Purified SLES (70% sol^n) : 1700 kg/day
- Processing losses & Degraded Components : 460 kg/day

...les of NaOH Consumed:

$$\frac{150\,kg/day}{40\,g/mol} = 3750\ mol/day$$

Total Heat Released:

$Q_4 = 3750 \times -57\ kJ/mol = -213{,}750\ kJ/day$

Heat Removal & Outlet Temperature:

Cp of SLES = 2.6 kJ/kg °C

$$\Delta T_4 = \frac{-213{,}750}{1860 \times 2.6} = -44.5\,°C$$

Outlet Temperature = 35°C (after cooling)

SLES Energy Balance -

Step-1: Hydrogenation of Palm Oil to Lauryl Alcohol

Reaction:

Palm Oil + H_2 ⟶ Lauryl Alcohol

Given data:

Reactant mass flow rate = 1200 kg/day

Hydrogen consumption = 30 kg/day

Typical hydrogenation reacⁿ enthalpy = −55 kJ/mol

Lauryl alcohol molar mass = 186.34 g/mol

Initial reactor temperature = 30°C

Catalyst: KOH

Moles of Lauryl Alcohol Produced:

$$\frac{980\ \text{kg/day}}{186.34\ \text{g/mol}} = 5260.7\ \text{mol/day}$$

Total Heat Released.

$$q_1 = 5260.7 \times -55\ \text{kJ/mol} = -289{,}338.5\ \text{kJ/day}$$

Heat Removal & Outlet Temperature:

C_p of Lauryl Alcohol = 2.1 kJ/kg°C.

$$\Delta T_1 = \frac{-289{,}338.5}{980 \times 2.1} = -141.9\,°C.$$

Since its exothermic, the reactor would require cooling to maintain reaction stability

Outlet Temperature = 30°C (after cooling).

Step-2: Ethoxylation of lauryl Alcohol

Reaction:

$C_{12}H_{20}O + n(C_2H_4O) \rightarrow C_{12}H_{26}(OCH_2CH_2)_nOH$

Given Data -

Reactant mass flow rate = 980 kg/day

Ethylene oxide consumption = 490 kg/day.

Typical ethoxylation reaction enthalpy = -120 kJ/mol

Initial temperature = 50°C.

Moles of Ethylene Oxide Consumed:

$\frac{490 \text{ kg/day}}{44.05 \text{ g/mol}} = 11,125.5 \text{ mol/day}$

Total Heat Released -

$Q_2 = 11,125.5 \times -120 \text{ kJ/mol} = -1,335,060 \text{ kJ/day}$

Heat Removal & Outlet Temperature:

Cp of lauryl Ether Alcohol = 2.5 kJ/kg°C.

$\Delta T_2 = \frac{-1,335,060}{1410 \times 2.5} \approx -370°C$

This step requires agressive cooling (jacked reactor with chilled water).

Outlet Temperature ≈ 50°C (Maintained by cooling)

Step-3: Sulfation of lauryl Ether Alcohol

Reaction:-

$C_{12}H_{26}(OCH_2CH_2)_3OH + SO_3 \rightarrow C_{12}H_{26}(OCH_2CH_2)_3OSO_3H$

Given Data:

Reactant mass flow rate = 1440 kg/day

SO_3 consumption = 360 kg/day

Typical sulfonation reaction ethalpy = -75 kJ/mol.

Initial Temp. = 40°C.

Moles of SO_3 consumed:

$$\frac{360\ \text{kg/day}}{80.06\ \text{g/mol}} = 4495.5\ \text{mol/day}$$

Total Heat Released:

$Q_3 = 4495.5 \times -75\ \text{kJ/mol} = -337,162.5\ \text{kJ/day}$

Heat Removal & Outlet Temperature.

Cp of Sulfated Product = 2.8 kJ/kg°C.

$$\Delta T_3 = \frac{-337,162.5}{1740 \times 2.8} = -69°C.$$

Outlet Temp. = 40°C (after controlled cooling)

Step-4 Neutralisation with NaOH

Reaction:

$C_{12}H_{26}(OCH_2CH_2)_3OSO_3H + NaOH \longrightarrow C_{12}H_{26}(OCH_2CH_2)_3OSO_3Na + H_2O$

Given Data:

Reactant mass flow rate = 1740 kg/day.

NaOH consumption = 150 kg/day.

Typical neutralization ethalpy = -57 kJ/mol.

Initial Temp. = 35°C.

Unit Operation	Heat Load (kJ/day)	Temp Change (ΔT, °C)	Outlet Temperature
Hydrogenation	−289,338.5	−141.9	30°C (controlled)
Ethoxylation	−1,335,060	−370	50°C (controlled)
Sulfation	−337,162.5	−69	40°C (controlled)
Neutralization	−213,750	−44.5	35°C (controlled)

(c) Evaluating capacity of reactors assuming only 70% of the total volume can be filled. For example, a 1000 L reactor can only fill 700 L reaction mixture.

Typical Density for reaction mixtures = 1.05 kg/L

(a) <u>Hydrogenation</u>

From the mass balance,

- Daily output = 980 kg/day (Lauryl Alcohol)
- Volume req. per day = $\frac{980\text{ kg/day}}{1.05\text{ kg/L}} \approx 933.33$ L/day

Since the reactor is used at 70% of total volume,

Volume of reactor = $\frac{933.33}{0.70} \approx 1,333.33$ L

So, reactor capacity for hydrogenation = 1,500 L

(b) <u>Ethyoxylation</u>

From the mass balance,

- Daily output = 1440 kg/day (Lauryl Ether Alcohol)
- Volume req. per day = $\frac{1440\text{ kg/day}}{1.05\text{ kg/L}} \approx 1371.43$ L/day

Since the reactor is used at 70% of total volume :

Volume of reactor = $\frac{1371.43}{0.7} \approx 1959.18$ L

So, reactor capacity for ethoxylation = 2,000 L

(c) Sulfation

From the mass balance:

- Daily output = 1740 kg/day (SLES Acid Form)
- Volume req. per day = $\frac{1740 \text{ kg/day}}{1.05 \text{ kg/L}} \approx 1657.14 \text{ L/day}$

Since the reactor is used at 70% of total volume,

$$\text{Volume of reactor} = \frac{1657.14}{0.7} \approx 2,367.34 \text{ L}$$

So, reactor size for sulfation = 2500 L.

(d) Neutralization

From the mass balance:

- Daily output = 1860 kg/day (Crude SLES)
- Volume required/day = $\frac{1860 \text{ kg/day}}{1.05 \text{ kg/L}} \approx 1771.43 \text{ L/day}$

Since the reactor is used at 70% of total volume,

$$\text{Volume of reactor} = \frac{1771.43}{0.7} \approx 2,530.61 \text{ L}$$

So, reactor size for neutralization = 2,600 L

Types of reactors and why we used them in the process.

Autoclave Reactor:

- Advantages/reasons:
    - High-pressure reaction (hydrogen gas involved)
    - Exothermic reaction → Requires cooling jacket or coil
    - Catalyst-based reaction → Requires agitation for uniform mixing

Jacketed Agitated Reactor:

- Advantages/reasons:
    - Strong exothermic reaction → Efficient heat removal needed
    - Requires continuous mixing to prevent localized overheating
    - Jacketed design allows precise temperature control

Jacketed Non-agitated Reactor:

- Advantages/reason:
    - Sulfation reaction generates moderate heat
    - No agitation required since SO_3 diffuses easily
    - Jacketed design for temperature control

Mixer/Settler:

- Advantages/reason:
  - Mild exothermic reaction
  - Requires simple mixing and cooling
  - No strong pressure or temperature swings

Capital cost (for the reactors):

Step	Type of Reactor	Material of Reactor	No. of units	Design Capacity (L)	Internal Pressure (in psi)	Cost/unit (in US$ for year 2014)	Total Cost (in US$ for year 2014)
Hydrogenation	Autoclave	Glass-lined CS	1	1500	450 (high)	185,000	185,000
Ethoxylation	Jacketed, Agitated	Glass-lined CS	1	2000	100 (moderate)	46,200	46,200
Sulfation	Jacketed, Non-Agitated	Glass-lined CS	1	2500	75 (low)	9,300	9,300
Neutralization	Mixer/Settler	Glass-lined CS	1	2600	15 (atmospheric)	143,000	143,000

References:

1. "Perry's Chemical Engineers' Handbook" (7th ed.) by R.H. Perry & D.W. Green. McGraw-Hill. Available online

2. "Shreve's Chemical Process Industries" (4th ed.) by R.N. Shreve & J.A. Brink. McGraw-Hill. Available on Archive.org

3. Cost Estimation for Reactors – http://www.matche.com/equipcost/Reactor.html

4. SLES Production Process Design – "Production of Sodium Lauryl Ether Sulfate (SLES) via Ethoxylation and Sulfation." Industrial Process Journal, 2023.

5. Environmental Clearance for a SLES Plant (18,000 T/Y) – Link
6. US Patent on Ethoxylation and Sulfation for SLES Production – Patent US5674938A on Google patents. https://patents.google.com/patent/US5674938A

List the contributions of each author:

➔ Pratyush Biswal

- ★ Performed the mass and energy balance for the process.
- ★ Researched and determined the most feasible Process Flow Diagram (PFD) based on previous studies and market analysis.
- ★ Gave the block diagram for the feasible process (as determined in the market analysis report). Listed all unit operations and process conditions.
- ★ Gave the material balance for a scaled-up process plant with capacity of 1000 kg/day. (If needed, simplified the calculations by stating assumptions).

→ Armaan Pratik Pasayat

- Estimated the Volume requirements and capacity of each Reactor.
- Researched and compared the uses of different types of reactors to decide the best suited ones for each step.
- Calculated the capital cost for each reactor from the link provided.
- Studied the exact reactions involved based on previous reports and verified the PFD from the references.

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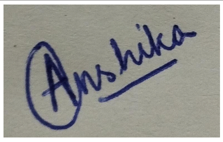
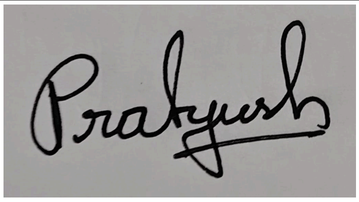
Anshika Agrawal	230160	
Pratyush Biswal	230783	
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