Technical Team

Nature of Invention: Process Flow Diagram and Mass Balance

Applicant: QuantiVEX

Inventors: Bipin Kumar Jaiswal, Nonit Gupta, Peeyush Sahu, Sarthak Singh

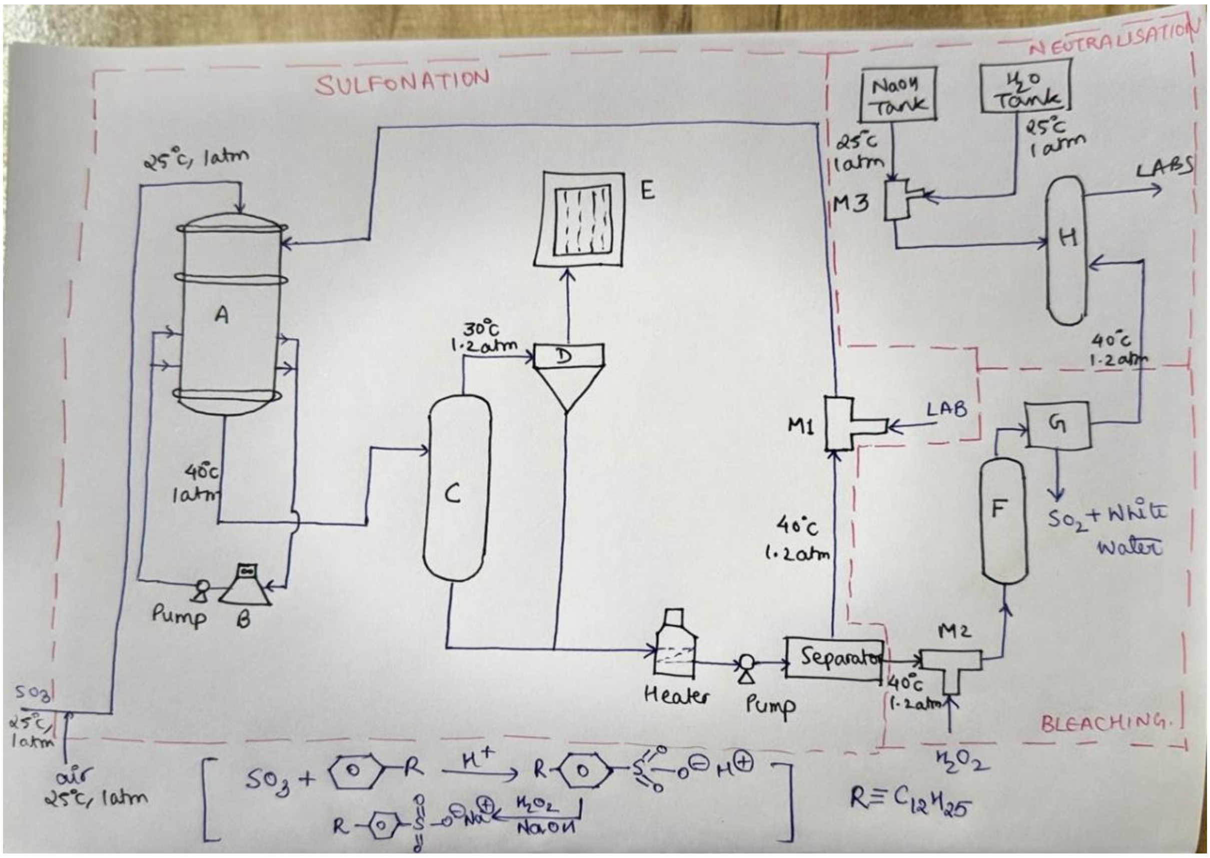
Chemical Formula: (R-C6H4-SO3Na)

Chemical Name: Linear alkyl benzene sulphonate

Process Title: Production of Linear alkyl benzene sulphonate from linear alkyl benzene

Process Description:

a. Process Flow Diagram:



where;

A → Falling Film Reactor

B → Cooling Tower

C → Separator

D → Cyclone

E → Electrostatic Precipitator

F → Bleaching Tower

G → Dilution Tank

H → Neutralization Vessel

M1, M2, M3 → Static Mixer

1 Reaction information

1.1 Main Reaction

$$C_6H_5-R+SO_3+NaOH \xrightarrow{H^+} C_6H_4-R-SO_3Na+H_2O$$

Here, we have taken the alkyl group $-R$ as C-12: $-(CH_2)_{11}CH_3$

1.2 Molecular Weights

Compound	Formula	Molecular Weight (kg/kmol)
Sulfonating Agent	SO_3	80.06
Linear Alkyl Benzene	C_6H_5-R	246.42
Linear Alkyl Benzene Sulfonic Acid	$C_6H_4-R-SO_3H$	326.48
Linear Alkyl Benzene Sulfonate	$C_6H_4-R-SO_3Na$	348.45

Table 1: Molecular Weights of LAB and its Sulfonation Products

2 Basis Calculations

We take the production of Linear Alkyl Benzene Sulfonate (LABS) as **1000 kg/day** with an **overall molar conversion of 90%**.

2.1 Calculation of Molar and Mass Flow Rates

Step 1: Calculate LABS Molar Flow Rate
The molar flow rate of LABS in kmol/hr:

$$\dot{n}_{\text{LABS}} = \frac{\text{Mass Flow Rate}}{\text{Molecular Weight}} = \frac{1000\ kg/day}{348.45\ kg/kmol} \times \frac{1}{24\ hr/day}$$

$$\dot{n}_{\text{LABS}} = 0.12\ kmol/hr$$

Step 2: Calculate Molar Flow Rate of LAB and SO_3 in Feed Stream
Since the overall molar conversion is **90%**, the required molar flow rates of reactants are:

$$\dot{n}_{\text{C}_6\text{H}_5\,-\,\text{R}} = \frac{\dot{n}_{\text{LABS}}}{\text{Conversion}} = \frac{0.12}{0.90} = 0.13\ kmol/hr$$

$$\dot{n}_{\text{SO}_3} = \dot{n}_{\text{C}_6\text{H}_5\,-\,\text{R}} = 0.13\ kmol/hr$$

Step 3: Calculate Mass Flow Rates of All Components
Using mass flow rate formula:

$$\dot{m} = \dot{n} \times M$$

$$\dot{m}_{\text{C}_6\text{H}_5\,-\,\text{R}} = 0.13 \times 246.42 = 32.03\ kg/hr$$
$$\dot{m}_{\text{SO}_3} = 0.13 \times 80.06 = 10.41\ kg/hr$$
$$\dot{m}_{\text{LABS}} = 0.12 \times 348.45 = 41.81\ kg/hr$$

2.2 Final Flow Rate Table

Component	Formula	Molar Flow Rate kmol/hr	Mass Flow Rate kg/hr
Linear Alkyl Benzene (LAB)	$C_6H_5 - R$	0.13	32.03
Sulfonating Agent	SO_3	0.13	10.41
Linear Alkyl Benzene Sulfonic Acid (LABSA)	$C_6H_4 - R - SO_3H$	0.12	41.81

Table 2: Molar and Mass Flow Rates of Reactants and Products

3 Mass Flow Balances

3.1 Falling-Film Reactor

Key Assumptions:

- **Overall Production Basis:** 1000 kg LABS/day, which is equivalent to:

$$41.81 \text{ kg/hr} = 0.12 \text{ kmol/hr LABS salt}$$

- **Single-Pass Conversion** (η): 90% (based on total LAB feed).
- **Recycle Efficiency** (r): 90% of unreacted LAB is recovered and recycled.

3.1.1 Step 1: Determine Required LAB Reaction to Meet Final Product

- From the stoichiometry, we assume:

  Moles of LABS salt produced = Moles of LABSA produced = Moles of LAB consumed

- Hence, for 100% conversion, the total LAB required:

$$F_{\text{total}} = 0.12 \text{ kmol/hr}$$

- Given that the single-pass conversion of LAB in the Falling-Film Reactor (FFR) is 90%:

$$F_{\text{total}} = \frac{0.12}{0.9} = 0.133 \text{ kmol/hr}$$

3.1.2 Step 2: Determine Unreacted LAB and Recycle Stream

- The molar flow rate of unreacted LAB:

$$F_{\text{unreacted}} = (1-\eta) \times F_{\text{total}} = 0.1 \times 0.133 = 0.013 \text{ kmol/hr}$$

- With a 95% recovery efficiency, the recycled LAB stream:

$$R = 0.9 \times F_{\text{unreacted}} = 0.9 \times 0.013 = 0.0117 \text{ kmol/hr}$$

3.1.3 Step 3: Determine the Required Fresh LAB Feed

- Using the mass balance equation: $F_{\text{total}} = F_{\text{fresh}} + R$
- Solving for F_{fresh}: $F_{\text{fresh}} = 0.133 - 0.0117 = 0.1213$ kmol/hr

3.1.4 Step 4: SO_3 Requirement in the Reactor

- The reaction follows a 1:1 molar ratio.
- Hence, the molar flow rate of SO_3 reacted:

$$F_{SO_3} = F_{\text{total}} \times \eta = 0.133 \times 0.9 = 0.1197 \text{ kmol/hr}$$

Summary of Molar and Mass Flow Rates

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Linear Alkyl Benzene Sulfonic Acid (LABSA)	-	39.18
Linear Alkyl Benzene (LAB)	32.77	3.2
Sulfur Trioxide (SO_3)	9.58	-
Total	**42.35**	**42.38**

Table 3: Summary of Mass Flow Rates in the Reactor

3.2 Bleaching

Reaction:
$\text{LABSA (dark coloured)} + H_2O_2 \longrightarrow \text{LABSA (light coloured)}$

- **Key Consideration:** The LABS itself remains chemically unchanged.
- During the bleaching process, impurities present in Linear Alkyl Benzene Sulfonic Acid (LABSA) react with a bleaching agent, such as hydrogen peroxide (H_2O_2) or sodium hypochlorite (NaOCl).
- This oxidation effectively removes color impurities without chemically altering the LABSA. Hence, mass flow rate of LABSA remains almost same.

3.3 Neutralization

Reaction:
$\text{LABSA} + \text{NaOH} \longrightarrow \text{LABS} + H_2O$

- **LABSA Neutralization:**
  - Input molar flow rate of LABSA = 0.12 kmol/hr
  - The reaction follows a 1:1 molar ratio. Hence,
    Molar flow rate of pure NaOH = 0.12 kmol/hr
- **NaOH Requirements:**
  - Mass flow rate of pure NaOH = $0.12 \times 39.997 = 4.8$ kg/hr
  - Given that typical NaOH aqueous solution is 30% w/w,
    Mass flow rate of NaOH solution = $\frac{4.8}{0.3} = 16$ kg/hr

- **Water Contributions:**
  - Water content from NaOH solution $= 16 - 4.8 = 11.2$ kg/hr
  - Water content from NaOH solution in molar terms $= \frac{11.2}{18} = 0.62$ kmol/hr
  - Water generated by the neutralization reaction $= 0.12$ kmol/hr
- **Total Water Output:**
  - Total water output $= 0.62 + 0.12 = 0.74$ kmol/hr
  - Mass flow rate $= 0.74 \times 18 = 13.32$ kg/hr

Summary of Mass Flows

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Linear Alkyl Benzene Sulfonate (LABS)	-	41.81
Linear Alkyl Benzene Sulfonic Acid (LABSA)	39.18	-
Sodium Hydroxide (NaOH)	4.8	-
Water (H_2O)	11.2	13.32
Total	**55.18**	**55.13**

Table 4: Mass Flow Summary of Compounds

4 Energy Balance

4.1 Falling-Film Reactor

Mass Flow Rates:

- Amount of SO_3 reacting: $\dot{m}_{\mathrm{SO_3}} = 9.58$ kg/hour
- Amount of LAB reacting: $\dot{m}_{\mathrm{LAB}} = 29.57$ kg/hour
- Amount of LABSA produced: $\dot{m}_{\mathrm{LABSA}} = 39.18$ kg/hour

Heat of Formation:

- SO_3: $\Delta H_{f,\mathrm{SO_3}} =$ -4.936 kJ/kg
- LAB: $\Delta H_{f,LAB} = 0.97$ kJ/kg
- LABSA: $\Delta H_{f,LABSA} =$ -0.53 kJ/kg

Heat of Reaction:

- $\Delta H_{rxn} = \dot{m}_{LABSA} \times \Delta H_{f,LABSA} + (\dot{m}_{\mathrm{SO_3}} \times \Delta H_{f,\mathrm{SO_3}} + \dot{m}_{LAB} \times \Delta H_{f,LAB})$
- Calculation:
  $\implies 39.18 \times -0.53 + (9.58 \times -4.936 + 29.57 \times 0.97) = -39.37$ kJ/hr

4.2 Heater

Mass Flow Rates:

- Mass flow rate of unreacted LAB: 0.32 kg/hr
- Mass flow rate of LABSA: 39.18 kg/hr

Specific Heat Capacity:

- LAB: 2.034 kJ/(kg.K)
- LABSA: 1.6 kJ/(kg.K)

Temperature Change:

- Inlet stream temperature: 30°C
- Outlet stream temperature: 40°C

Heat Input:

- $\dot{Q}_{in} = \dot{m}_{LAB} \times C_{P,LAB} \times \Delta T + \dot{m}_{LABSA} \times C_{P,LABSA} \times \Delta T$
- Calculation:
  $\implies 0.32 \times 2.034 \times 10 + 39.18 \times 1.6 \times 10 = 633.39$ kJ/hr

4.3 Neutralization

Heat of Reaction:

- Heat of neutralization: 55.9 kJ/mol

Molar Flow Rate:

- LABSA: 0.12 kmol/hr

Total Heat Released:

- $\Delta H_{neutralization} = 0.12 \times 1000 \times 55.9 = 6708$ kJ/hr

4.4 Overall Balance

- $\dot{Q}_{net} = \Delta H_{rxn} + \dot{Q}_{in} + \Delta H_{neutralization}$
- Calculation:
  $\implies -39.37 + 633.39 + 6708 = 7302.02$ kJ/hr

Capital cost (only for the reactor):

Equipment	Design Capacity (gallons)	No. of units	Cost/unit ($ for year 2014)	Total Cost ($ for year 2014)
Reactor A (Jacketed reactor & Agitated)	1800	1	64100	64100
Reactor H (Kettle,jacketed & Agitated)	39.63	1	38200	38200

References: Provided reference for a research paper or an actual patent.

1. http://www.matche.com/equipcost/Reactor.html
2. https://labsaco.com/labs-formula/ - LABSA properties (bleaching)
3. https://patents.google.com/patent/EP3146034A1/en - Neutralization of LABSA to form LABS.
4. https://iitk-my.sharepoint.com/:w:/g/personal/shubhamsg23_iitk_ac_in/EVMhAlWPa7dNvKlfeeYHFqABeJ6-Gd8LeL-QBXm8tM8qcw?e=Nr6U5Y

List the contributions of each author:

- **Process flow diagram:** Sarthak Singh
- **Material Balance:** Bipin Kumar Jaiswal,Nonit Gupta,Peeyush Sahu
- **Energy Balance:** Bipin Kumar Jaiswal,Nonit Gupta,Peeyush Sahu
- **Capital Cost:** Bipin Kumar Jaiswal

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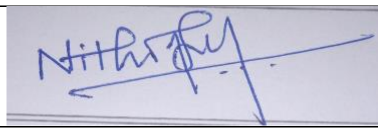
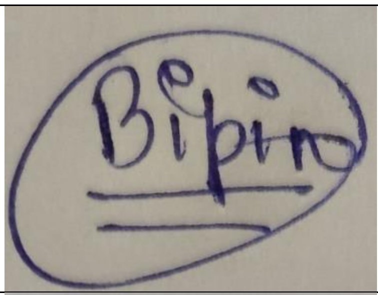
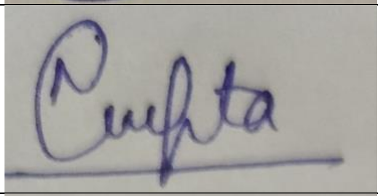
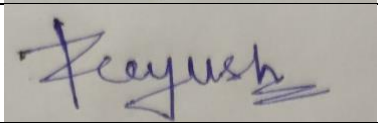
Nithin TM (CEO)	230709	

Bipin Kumar Jaiswal	230300	
Nonit Gupta	230712	
Peeyush Sahu	230750	
Sarthak Singh	230930