QuantiVEX
Technical Analysis Report
Linear Alkyl Benzene Sulphonate (LABS)

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March 24, 2025

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)**
Sulphonating Agent	SO_3	80.06
Linear Alkyl Benzene	C_6H_5-R	246.42
Linear Alkyl Benzene Sulphonic Acid	$C_6H_4-R-SO_3H$	326.48
Linear Alkyl Benzene Sulphonate	$C_6H_4-R-SO_3Na$	348.45

Table 1: Molecular Weights of LAB and its Sulfonation Products

2 Basis Calculations

We take the production of Linear Alkyl Benzene Sulphonate (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:

$$\dot{n}_{C_6H_5\,-\,R} = \frac{\dot{n}_{\text{LABS}}}{\text{Conversion}} = \frac{0.12}{0.90} = 0.13\ kmol/hr$$

$$\dot{n}_{SO_3} = \dot{n}_{C_6H_5\,-\,R} = 0.13\ kmol/hr$$

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

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

$$\begin{aligned}\dot{m}_{C_6H_5\,-\,R} &= 0.13 \times 246.42 = 32.03\ kg/hr\\ \dot{m}_{SO_3} &= 0.13 \times 80.06 = 10.41\ kg/hr\\ \dot{m}_{\text{LABS}} &= 0.12 \times 348.45 = 41.81\ kg/hr\end{aligned}$$

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
Sulphonating Agent	SO_3	0.13	10.41
Linear Alkyl Benzene Sulphonic 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 Balance across 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:

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

3.2 Summary of Molar Flow Rates

Component	**Molar Flow Rate (kmol/hr)**
LABS (Final Product)	0.12
Total LAB Feed (F_{total})	0.133
Fresh LAB Feed (F_{fresh})	0.1213
Unreacted LAB ($F_{\text{unreacted}}$)	0.013
Recycle LAB (R)	0.0117
SO_3 Required	0.1197

Table 3: Summary of Molar Flow Rates in the Reactor