

# QuantiVEX

## Technical Analysis Report

### Linear Alkyl Benzene Sulphonate (LABS)

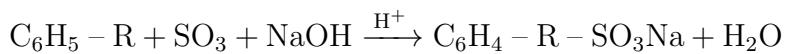
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## 1 Reaction information

### 1.1 Main Reaction



Here, we have taken the alkyl group  $- \text{R}$  as C-12:  $- (\text{CH}_2)_{11}\text{CH}_3$

### 1.2 Molecular Weights

Compound	Formula	Molecular Weight (kg/kmol)
Sulphonating Agent	$\text{SO}_3$	80.06
Linear Alkyl Benzene	$\text{C}_6\text{H}_5 - \text{R}$	246.42
Linear Alkyl Benzene Sulphonic Acid	$\text{C}_6\text{H}_4 - \text{R} - \text{SO}_3\text{H}$	326.48
Linear Alkyl Benzene Sulphonate	$\text{C}_6\text{H}_4 - \text{R} - \text{SO}_3\text{Na}$	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:

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

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

### Step 2: Calculate Molar Flow Rate of LAB and SO<sub>3</sub> in Feed Stream

Since the overall molar conversion is 90%, the required molar flow rates of reactants are:

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

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

### Step 3: Calculate Mass Flow Rates of All Components

Using mass flow rate formula:

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

$$\dot{m}_{\text{C}_6\text{H}_5 - \text{R}} = 0.13 \times 246.42 = 32.03 \text{ kg/hr}$$

$$\dot{m}_{\text{SO}_3} = 0.13 \times 80.06 = 10.41 \text{ kg/hr}$$

$$\dot{m}_{\text{LABS}} = 0.12 \times 348.45 = 41.81 \text{ kg/hr}$$

## 2.2 Final Flow Rate Table

Component	Formula	Molar Flow Rate kmol/hr	Mass Flow Rate kg/hr
Linear Alkyl Benzene (LAB)	C <sub>6</sub> H <sub>5</sub> – R	0.13	32.03
Sulphonating Agent	SO <sub>3</sub>	0.13	10.41
Linear Alkyl Benzene Sulphonic Acid (LABSA)	C <sub>6</sub> H <sub>4</sub> – R – SO <sub>3</sub> H	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 ( $\eta$ ): 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  $F_{\text{fresh}}$ :  $F_{\text{fresh}} = 0.133 - 0.0117 = 0.1213 \text{ kmol/hr}$

### 3.1.4 Step 4: SO<sub>3</sub> Requirement in the Reactor

- The reaction follows a 1:1 molar ratio.
- Hence, the molar flow rate of SO<sub>3</sub> reacted:

$$F_{\text{SO}_3} = F_{\text{total}} \times \eta = 0.133 \times 0.9 = 0.1197 \text{ kmol/hr}$$

### 3.2 Summary of Molar Flow Rates

Component	Molar Flow Rate (kmol/hr)
LABS (Final Product)	0.12
Total LAB Feed ( $F_{\text{total}}$ )	0.133
Fresh LAB Feed ( $F_{\text{fresh}}$ )	0.1213
Unreacted LAB ( $F_{\text{unreacted}}$ )	0.013
Recycle LAB ( $R$ )	0.0117
SO <sub>3</sub> Required	0.1197

Table 3: Summary of Molar Flow Rates in the Reactor