

# QuantiVEX

Quantifying Chemistry. Qualifying Tomorrow.

## Business Presentation

# TEAM

Pulkit  
Aditya  
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R&D

MARKET

Sarthak  
Bipin  
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TECHNICAL

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Sajag  
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Om Singh

**QUANTIVEX**

(CEO : Nithin T M)

# **VISION**

To become a leading innovator in chemical evaluation and industrial research, driving the future of sustainable process design and chemical intelligence.

# **MISSION**

To deliver high-quality, data-driven chemical analysis that empowers industries with safe, efficient, and sustainable solutions.

# R & D

## ***R&D Team :***

- Pulkit
- Aditya Nitin Patil
- Nithin D H
- Shubham Singh

# Patent on FAE (Fatty Acid Ethoxylates)

## OVERVIEW OF FAE SYNTHESIS

Uses: Green Synthesis of Fatty Acid Esters – Biodegradable Nonionic Surfactants

*Chemical Family:* Fatty Acid Ethoxylates (FAEs)

*General Formula:* R-COO-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>n</sub>-R'

R: Fatty acid chain (C<sub>12</sub>-C<sub>18</sub>)

R': Alcohol end (ethanol, glycerol, etc.)

n: Degree of ethoxylation (1-20)

yield-92-95%;

*Applications:* Detergents, emulsifiers, fabric softeners, agrochemicals

, Biodegradable + eco-friendly alternative to conventional surfactants

USP: Low toxicity, high wetting & emulsifying ability

# ENZYMATIC SYNTHESIS ROUTE

*Reaction:* Fatty Acid + Alcohol  $\rightleftharpoons$  Fatty Acid Ester + Water

*Catalyst:* Lipase enzyme (e.g. *Candida antarctica*)

*Temperature:* 35–60°C

Solvent-free or green solvent medium

Vacuum used to shift equilibrium by removing water

## *Process Highlights:*

Mild conditions → energy-efficient

High selectivity → minimal byproducts

Recyclable enzymes (immobilized)

- *Typical Esters:* Methyl Oleate, Ethyl Palmitate, Glycerol Stearate

# ACID-CATALYZED ESTERIFICATION (ALTERNATE)

*Acid-Catalyzed Esterification  
(Alternate)*

*Catalyst: Sulfuric acid / p-TSA  
Conditions: 120–150°C, ~3–4 hr*

## Drawbacks:

Acidic waste stream → Neutralization required

Side reactions → Dark color, degradation

Lower purity, high post-treatment effort

Higher E-factor (3)(waste generation index)

## Conclusion:

- >Enzyme-based synthesis = cleaner, safer, and industry-scalable
- >Acid route = waste-heavy and harsh

# Patent on Sodium Lauroyl Sarcosinate

## OVERVIEW OF INVENTION

Uses: A Mild, Biodegradable Surfactant

Chemical Information:

- Chemical Name: Sodium N-Lauroyl Sarcosinate
- Formula:  $C_{15}H_{28}NNaO_3$  | M.W.: ~293.38 g/mol
- Structure:  $CH_3-(CH_2)_{10}-C(=O)-N(CH_3)-CH_2-COO^- Na^+$
- Appearance: White powder or liquid
- pH (5%): 7.0–8.5 | Solubility: Fully water-soluble
- Uses: Personal care (shampoos, cleansers), mild foaming agent

USP: High biodegradability + gentle on skin

# DIRECT AMIDATION PROCESS

## *Key Raw Materials:*

- Lauric Acid, Sarcosine, NaOH, Catalyst (Lipase/NaOH), Solvent

## *Steps:*

- **Amidation** (80–120°C):



- Base/enzyme catalysis

- Water removed via evaporation

- **Neutralization:**



- pH adjusted to 8.5–9

- Final drying/spray drying

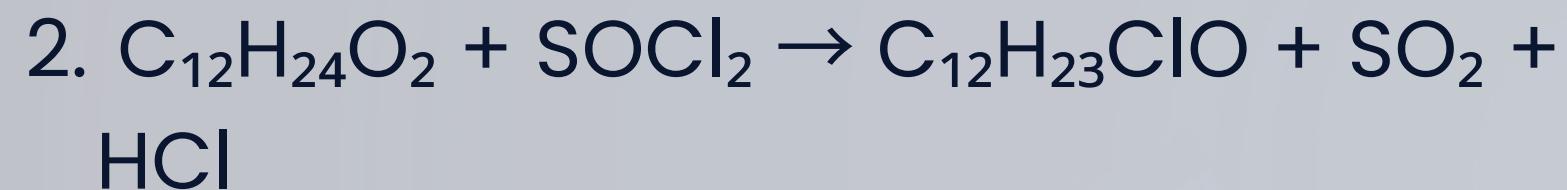
- Yield: ~95% | Purity: >99% | Eco-friendly

- Equipment: Reactor, distillation, scrubbers, DCS/PLC

# ACID CHLORIDE ROUTE (ALTERNATE)

## Steps:

1. Lauroyl Chloride Formation:



- Toxic byproducts → gas scrubbing needed

3. Amidation with Sarcosine:



5. Neutralization:



## Cons:

- Uses hazardous  $SOCl_2$
- Lower yield (~85%), intensive purification
- Requires solvent removal, filtration, extraction, crystallization

Conclusion: Direct Amidation is safer, greener & more efficient

# Patent on LABS

## OVERVIEW OF INVENTION

Uses: Linear Alkyl Benzene Sulfonate – The Workhorse of Anionic Surfactants

Chemical Formula: R-C<sub>6</sub>H<sub>4</sub>-SO<sub>3</sub>Na

R: Linear alkyl chain (C<sub>10</sub>-C<sub>14</sub>)

*Properties:*

High foaming, excellent detergency, good emulsifying power

Biodegradable (linear chain advantage)

Anionic surfactant, widely used in detergents

yield-98%;

*Applications:*

Laundry detergents, dishwashing liquids, industrial cleaners

Textile auxiliaries, agrochemical emulsifiers

# LABS MANUFACTURING – KEY STEPS

## *Alkylation:*

Linear alkyl group (e.g. n-dodecane) + Benzene → Linear Alkyl Benzene (LAB)

Catalyst: HF /  $\text{AlCl}_3$  / Zeolite

Selectivity for 2-phenyl isomer preferred for biodegradability

## *Sulfonation:*

LAB +  $\text{SO}_3$  → LAB Sulfonic Acid

Continuous film reactor or falling film sulfonator

Controlled to avoid disulfonation

## *Neutralization:*

LABSA + NaOH → LABS (sodium salt) +  $\text{H}_2\text{O}$

## *Key Equipment:*

- Alkylation reactor, sulfonator, scrubbers, neutralizer

# Process Comparison & Green Aspects

Parameter	HF catalyst route	Zeolite Catalyst route
Catalyst handling	Corrosive, toxic	safe, solid, recyclable
Selectivity(2-phenyl)	~70%	Up to 90%
Environmental Impact	High	Low
Cost	Moderate	Slightly higher Initially

## Conclusion:

Zeolite-based alkylation + SO<sub>3</sub> sulfonation = best industrial practice

Cleaner emissions, less corrosive, safer for plant operations

LABS remains a cornerstone surfactant due to its cost-performance balance

# MARKET ANALYSIS

***Market Team :***

- Sajag
- Shivam
- Venugopal
- Priyanka

***Report Submitted for :***

- 1) Fatty alcohol ethoxylates
- 2) Linear alkyl benzene sulphonate

# FAE

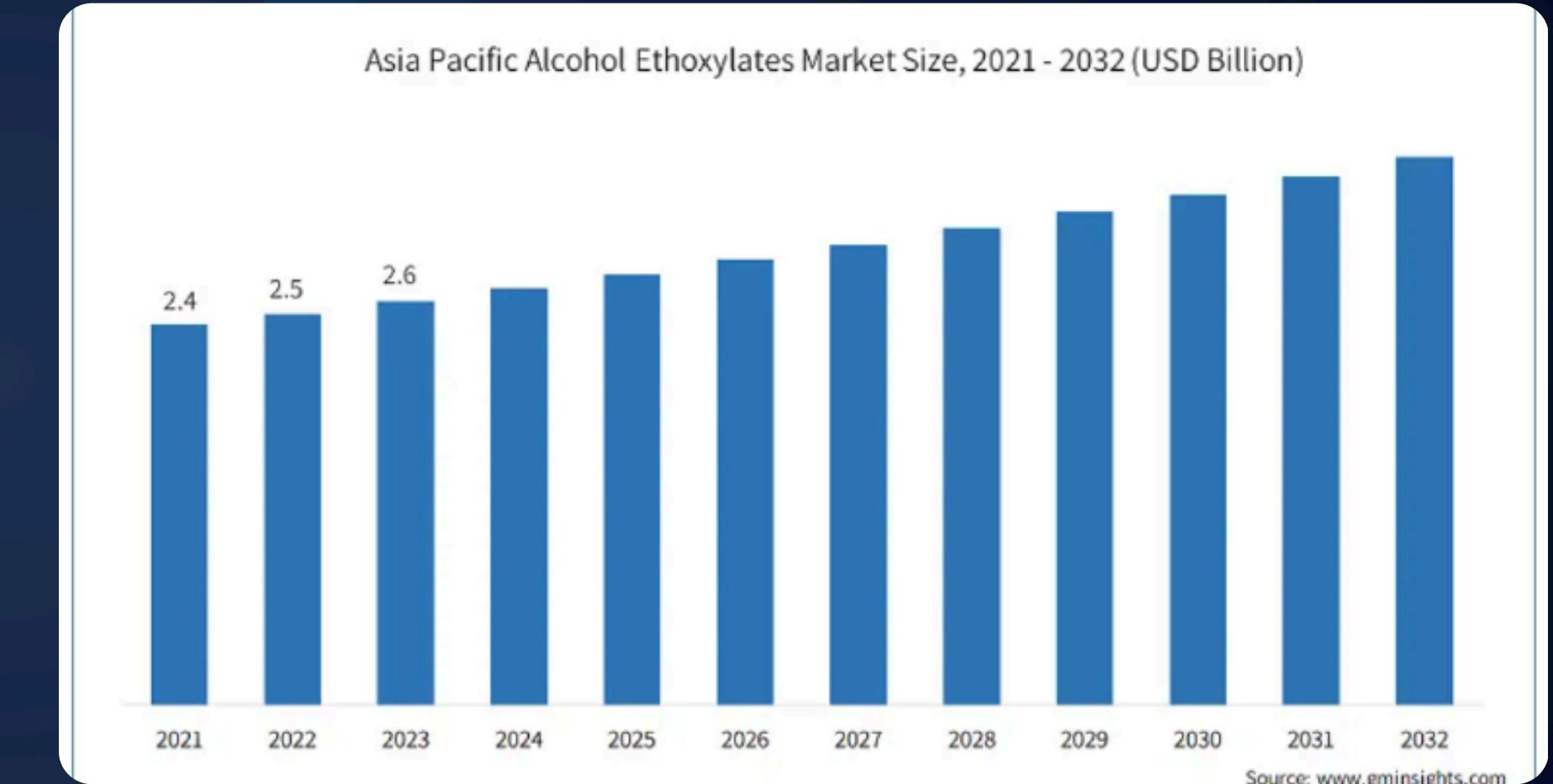
## ***FAE – Market Overview***

- Definition: Non-ionic surfactants used in detergents, personal care, and industrial cleaning.
- Global Market Size (2023): ~\$4.5 billion
- Expected CAGR (2024–2030): ~5 - 7%
- Applications: Shampoos, surface cleaners, textile scouring agents

## FAE - Key Regions & Players

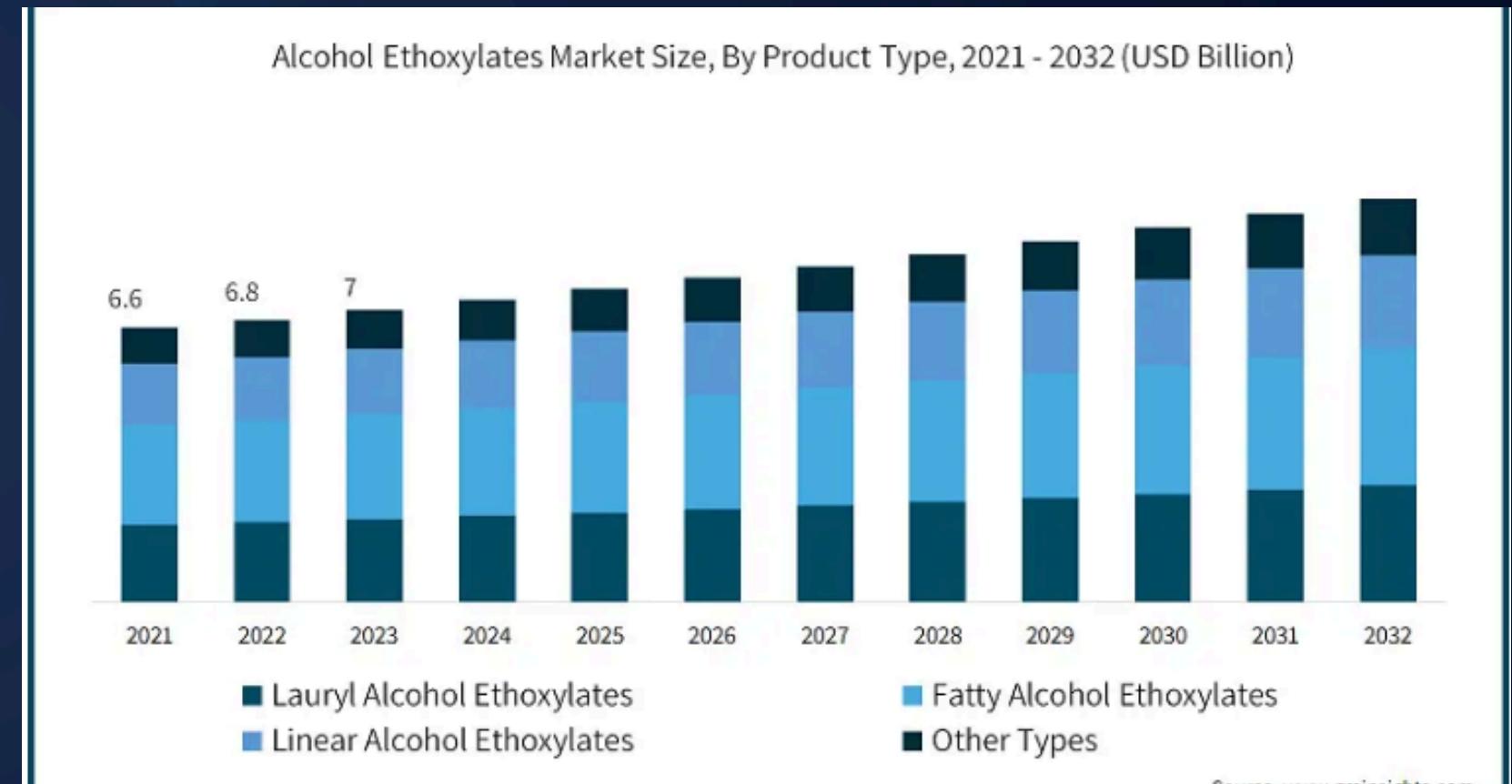
- Leading Producers: *BASF, Clariant, Croda, Huntsman, Sasol*
- Domestic Producers: WF India Ltd., Godrej Industries, Esteem Industries, Stepan India Private Ltd., Galaxy Surfactants Ltd.
- Production Hotspots:
  - Asia-Pacific (*China, India dominate production*)
  - Europe & North America (*tech innovation focus*)

Asia Pacific Alcohol Ethoxylates Market Size, 2021 - 2032 (USD Billion)



## FAE - Trends & Opportunities

- Emerging Trends:
  - Demand for natural-source ethoxylates (e.g., palm, coconut)
  - Biodegradability emphasis
- Opportunities:
  - Growth in personal care
  - Institutional cleaning in APAC & Africa
- Challenges: EO handling, raw material cost volatility
- Profit( 1 metric tone) : **3.7 Cr/yr**
- Gross Profit Margin:  $(₹102.4/₹250) \times 100 = 40.9\%$
- ROI : 22.3%, payback period : 4.5 years



# LABS

## ***LABS – Market Overview***

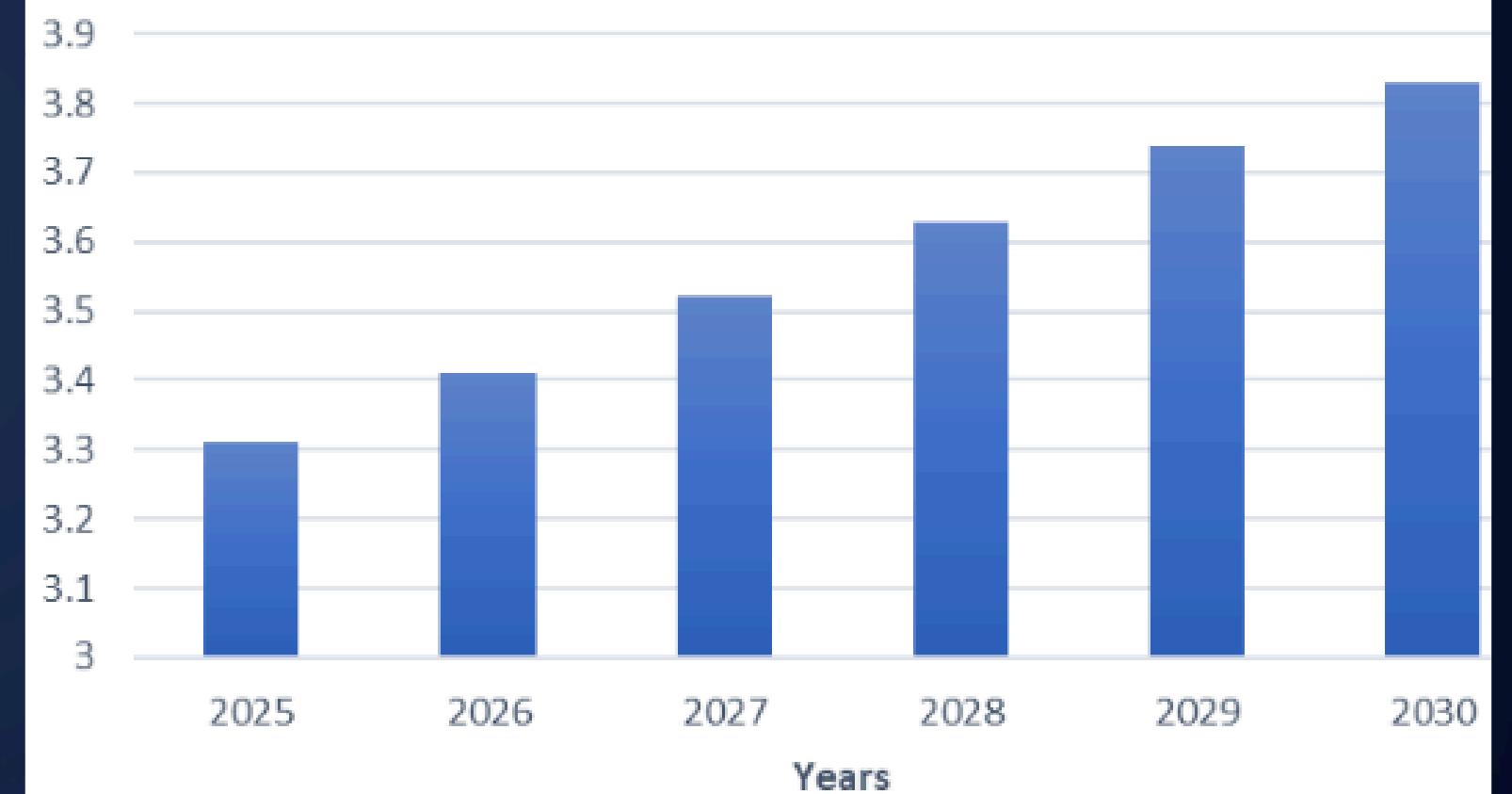
- *Definition: Anionic surfactant in detergents and household cleaning*
- *Market Size (2023): ~\$10.1 billion*
- *Expected CAGR (2024–2029): ~3.8%*
- *Applications: Laundry, dishwashing liquids, industrial cleaners, Leather industry, Paper industry*

# LABS

## LABS - Production & Demand

- Raw Inputs: LAB (from kerosene), SO<sub>3</sub>
- Top Producers: Stepan, CEPSA, ISU Chemical, Reliance
- India Insight: Demand CAGR >5%, policy push for self-sufficiency
- Profit( 1 metric ton) : **2.25 Cr/yr**
- Gross Profit Margin % =  $(69.48 / 140) \times 100 = 49.62\%$
- ROI of 16.5%, payback period of 6 years

CAGR for LABS (worldwide)



# LABS

## LABS - Trends & Challenges

- *Trends:*
  - *Rise in concentrated detergent formats*
  - *Move toward environmentally friendly LABS*
- *Challenges:*
  - *Price volatility (LAB/raw materials dependence )*
  - *Regulatory pressure on water safety*

### Major Exporter of LABS in India:

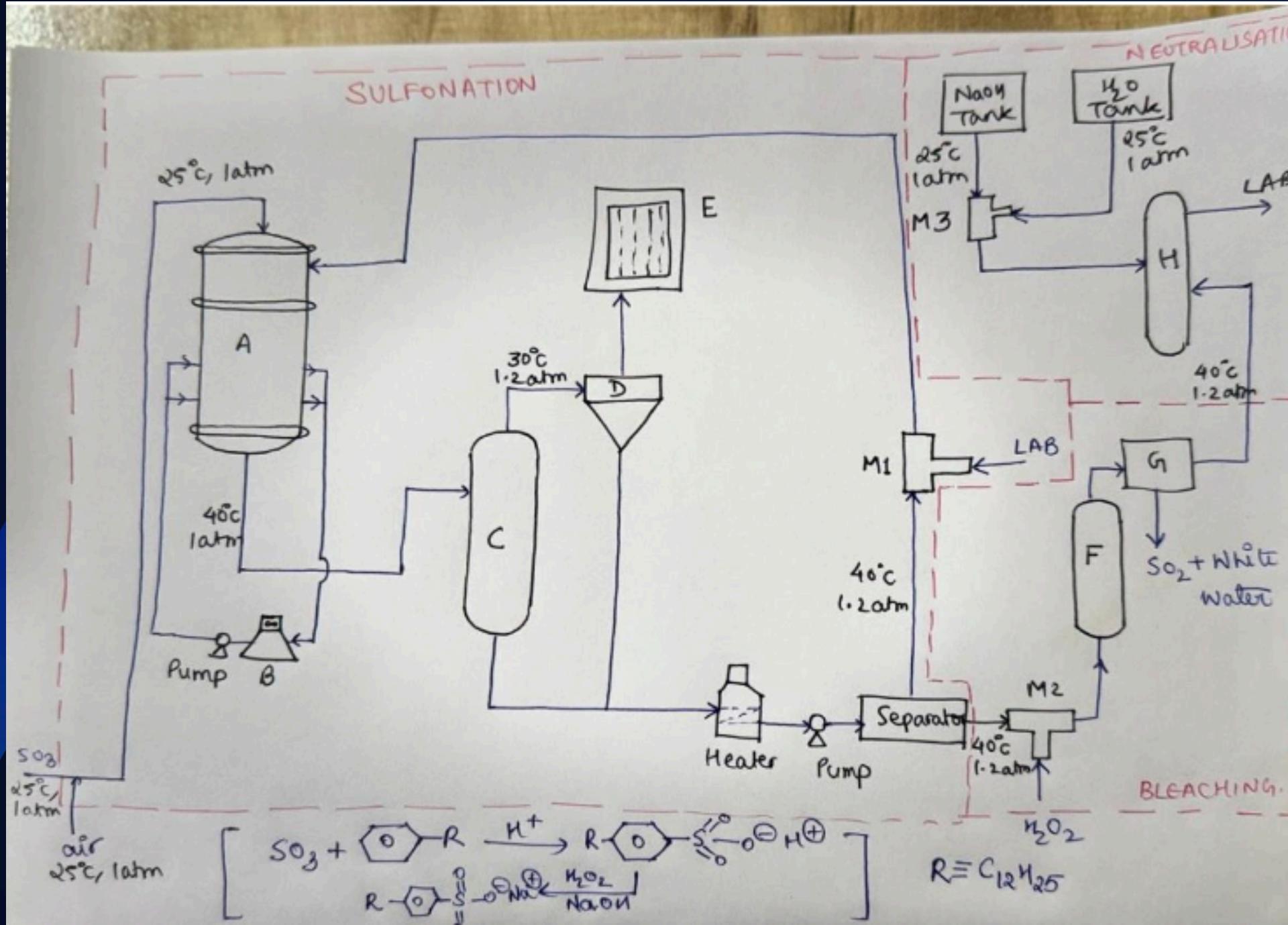
Name	Annual Export Value (in millions USD)	Key Destinations	Quantity (MT/year)
Nirma Ltd.	80 - 100	Vietnam, UAE, Egypt ,Brazil, South Africa	60,000 - 80,000
Tamilnadu Petroproducts Ltd	50 -70	Turkey, Indonesia, Nigeria, Iraq	40,000 - 60,000
Re Reliance Industries Ltd.	30 - 50	Bangladesh, Sri Lanka, Kenya, Iran	20,000 - 30,000
Galaxy Surfactants	20 - 30	Philippines, Morocco ,Saudi Arabia	15,000 - 20,000
Hexa Chemical	10 -15	Malaysia, Thailand, Egypt	8,000 - 12,000

# TECHNICAL TEAM

- *Sarthak Singh*
- *Bipin Kumar Jaiswal*
- *Nonit Gupta*
- *Peeyush Sahu*

# LABS

## Process FlowSheet



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

# LABS

## 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

## 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	-
<b>Total</b>	<b>42.35</b>	<b>42.38</b>

Table 3: Summary of Mass Flow Rates in the Reactor

# LABS

## 3.2 Bleaching

Reaction:



- **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 ( $\text{H}_2\text{O}_2$ ) or sodium hypochlorite ( $\text{NaOCl}$ ).
- This oxidation effectively removes color impurities without chemically altering the LABSA. Hence, mass flow rate of LABSA remains almost same.

### 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 ( $\text{H}_2\text{O}$ )	11.2	13.32
<b>Total</b>	<b>55.18</b>	<b>55.13</b>

Table 4: Mass Flow Summary of Compounds

# LABS

## Energy Requirements:

### 4.4 Overall Balance

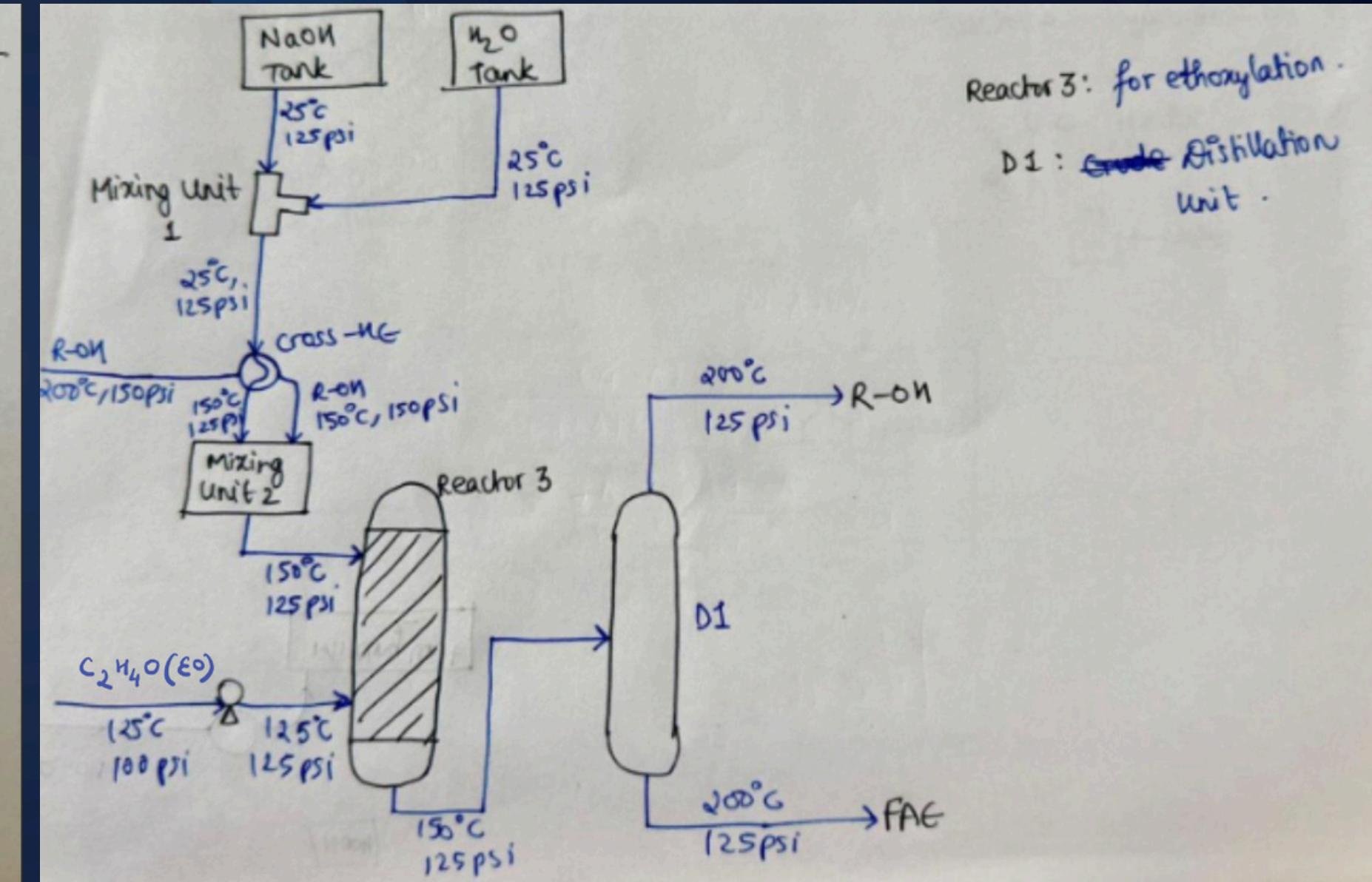
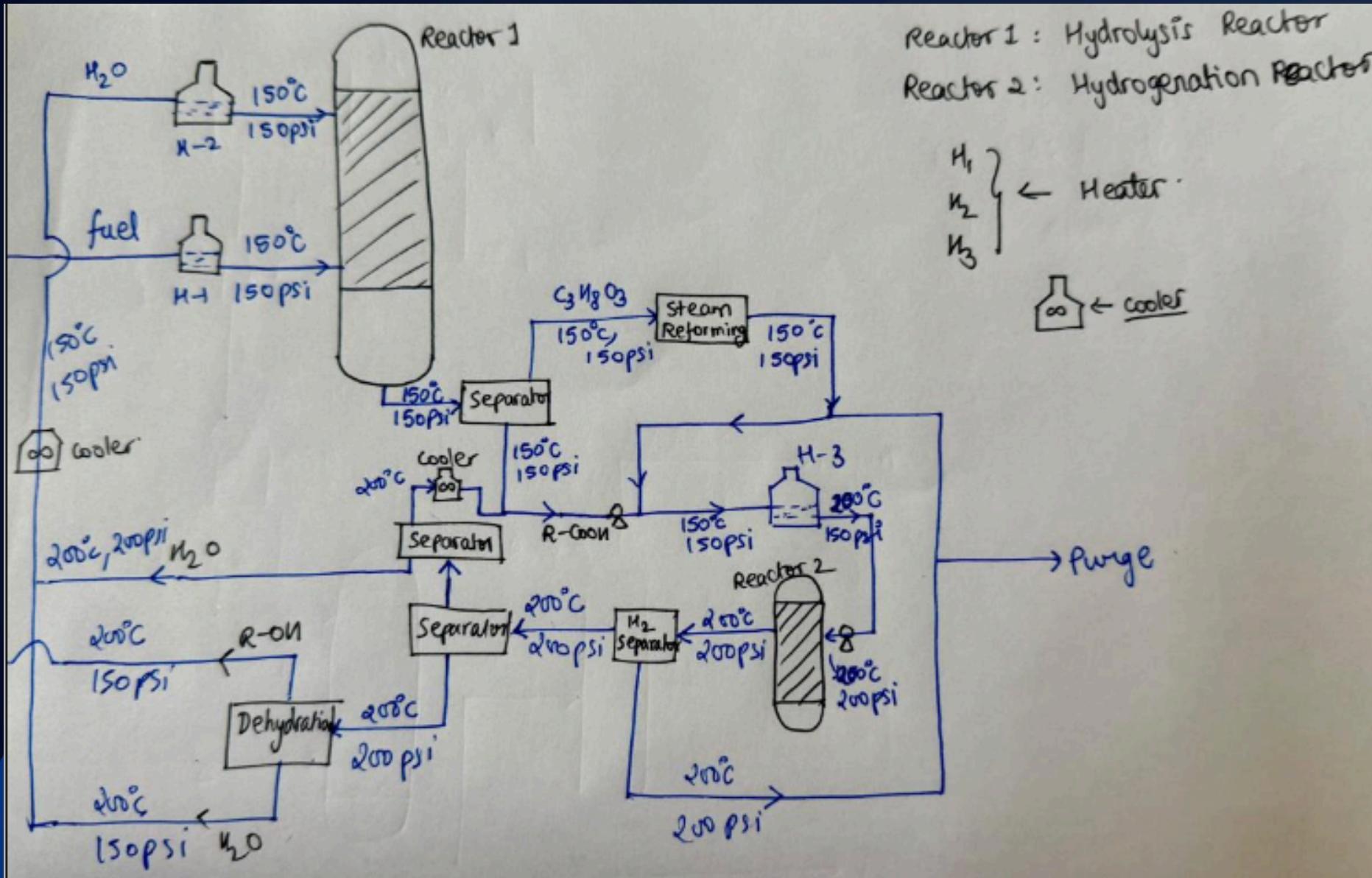
- $\dot{Q}_{net} = \Delta H_{rxn} + \dot{Q}_{in} + \Delta H_{neutralization}$
- Calculation:  
 $\Rightarrow -39.37 + 633.39 + 6708 = 7302.02 \text{ kJ/hr}$

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

# FAE

## Process FlowSheet



# FAE

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Triglycerides	28.53	1.43
Water	1.728	0.086
Fatty Acid	-	25.94
Glycerol	-	2.80
<b>Total</b>	<b>30.26</b>	<b>30.26</b>

Table 2: Mass Flow Summary of Compounds in Hydrolysis of Triglycerides

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Glycerol	2.80	-
Water	1.64	-
Hydrogen	-	0.43
Carbon Dioxide	-	4.01
<b>Total</b>	<b>4.44</b>	<b>4.44</b>

Table 3: Mass Flow Summary of Compounds in Steam Reforming of Glycerol

# FAE

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Fatty acids	25.94	1.27
Hydrogen	0.35	0.10
Fatty alcohol	-	23.46
Water	-	1.56
<b>Total</b>	<b>26.3</b>	<b>26.4</b>

Table 4: Mass Flow Summary of Compounds in Hydrogenation of Fatty Acids

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Fatty alcohol	23.46	-
Sodium Hydroxide	3.47	-
Alkoxide	-	25.37
Water	-	1.56
<b>Total</b>	<b>26.93</b>	<b>26.93</b>

Table 5: Mass Flow Summary of Compounds in Alkoxide Formation

# FAE

Compound Name	In Mass Flow (kg/hr)	Out Mass Flow (kg/hr)
Alkoxide	25.37	-
Ethylene Oxide	19.10	-
Water	1.56	-
Fatty Alcohol Ethoxylates	-	42.56
Sodium Hydroxide	-	3.47
<b>Total</b>	<b>46.03</b>	<b>46.03</b>

Table 6: Mass Flow Summary of Compounds in Ethoxylation

Energy  
requirements:

## 4.3 Total Heat Given or Consumed

The total energy input/output in the process is calculated as:

$$\dot{Q}_{net} = \sum \dot{Q}_{in} - \sum \dot{Q}_{out} \quad (\text{kJ/hour})$$

$$\Rightarrow \dot{Q}_{net} = 13605.39 - 1041.90 = 12563.49 \text{ kJ/hr}$$

# FAE

## Capital Cost Estimation :

Equipment	Design Capacity (L)	No. of units	Cost/unit (\$ for year 2014)	Total Cost (\$ for year 2014)
REACTOR 1  (Jacketed reactor, agitated, Carbon steel, pressure of 150 psi)	2000	1	39,500	39,500
REACTOR 2  (Jacketed, agitated, carbon steel, pressure of 300 psi)	1000	1	37,100	37,100
REACTOR 3  (Jacketed, agitated, carbon steel, pressure of 150 psi)	1000	1	25,600	25,600

# EHS TEAM

- Arnav Harshit
- Om Jee Singh

# LABS

## WHY LABS WAS CHOSEN OVER OTHER CHEMICALS ?

- Widely Used Surfactant: LABS is the most common anionic surfactant globally, essential in both household and industrial detergents.
- Environmental Compatibility: Biodegradable and eco-friendlier than older surfactants like alkylphenol ethoxylates.
- Versatile Application: Effective in both hard and soft water, making it suitable for a broad market.
- Established Industrial Process: Well-understood manufacturing with scope for EHS optimization.
- Patentability & Market Potential: Opportunities for innovation in waste minimization, energy optimization, and process safety.

# LABS

## WASTE GENERATION IN LABS PRODUCTION:

*Key Waste Streams per kg of LABS:*

- Residual  $H_2SO_4$ : 0.01–0.02 kg
- Unreacted LAB: ~0.01 kg
- Wastewater (neutralization, washing): 0.8–1.5 kg
- $SO_2, SO_3$  Emissions: <0.05 kg
- VOCs: ~0.01 kg (includes benzene traces)
- *E-factor = 1.59*

## Regulatory Limits & Disposal Standards

Waste Component	Regulatory Limit (ppm)	Disposal Method
Sulfuric Acid ( $H_2SO_4$ )	<100 ppm in effluent	Neutralization & Recycling
LAB Residue	Should not exceed 0.1% in final product	Recycle in process
Wastewater BOD	<30 ppm	Treatment via activated carbon
SOx Emissions	<500 mg/m <sup>3</sup>	Scrubbing & Adsorption
VOCs	<10 ppm	Adsorption on Activated Carbon

# LABS

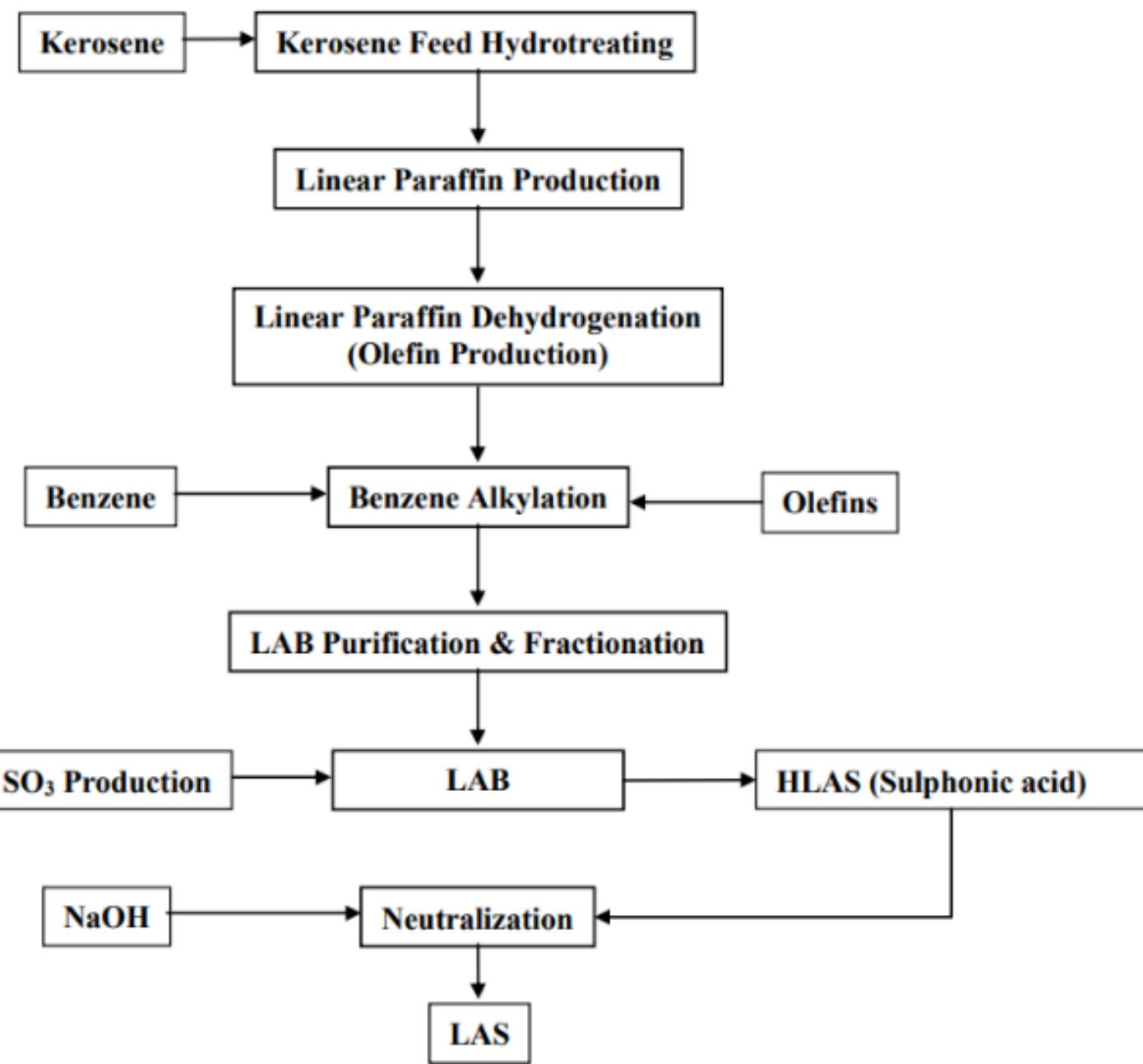
## WASTE TREATMENT AND ZERO LIQUID DISCHARGE (ZLD):

- Acid Recovery:  $\text{H}_2\text{SO}_4$  neutralized with  $\text{NaOH}/\text{Ca}(\text{OH})_2 \rightarrow \text{Na}_2\text{SO}_4/\text{CaSO}_4$  reused in cement industry.
- Water Treatment:
  - > Primary: Filtration, sedimentation.
  - > Secondary: Activated sludge process.
  - > Tertiary: Reverse osmosis → ZLD achieved.
- Air Emission Control:
  - > SOx: Scrubbed with lime slurry or  $\text{NH}_3$ .
  - > VOCs: Removed using activated carbon & biofiltration.

# LABS

## PROCESSING STEPS

Processing Steps in LAB-LAS Production



## Occupational Exposure Limits (OELs)

Chemical	TWA(8hr)	STEL(15min)	Health Risks
Sulfuric Acid (H <sub>2</sub> SO <sub>4</sub> )	1 mg/m <sup>3</sup>	3 mg/m <sup>3</sup>	Skin & eye irritation, respiratory issues
LAB Vapors	5 ppm	10 ppm	Irritation, dizziness, long-term exposure risks
Benzene (Trace)	0.5 ppm	2.5 ppm	Carcinogenic, bone marrow suppression
VOCs (General)	50 ppm	100 ppm	Neurological effects, respiratory issues

# LABS

## HEALTH, SAFETY & RISK MITIGATION:

- OELs & Health Risks:
  - > $\text{H}_2\text{SO}_4$ : Eye/respiratory irritation.
  - >LAB & VOCs: Dizziness, long-term exposure issues.
  - >Benzene (trace): Carcinogenic.
- PPE Requirements: Full-body protection, N95 masks, eye/face shields.
- Risk Controls:
  - >Spill kits, scrubbers for acidic vapors.
  - >Real-time leak detection, automated fire suppression.
  - >Emergency protocols for spills and VOC inhalation.

# LABS

## SUSTAINABILITY & RECOMMENDATIONS:

### *Green Chemistry Integration:*

- Exploring bio-based LABS alternatives.
- Implementing waste heat recovery.
- Using renewable energy to cut emissions.

### *Process Optimization Suggestions:*

- Adopt closed-loop water systems.
- Improve scrubber efficiency (multi-stage systems).
- Strengthen real-time monitoring for safety and compliance.

### *Compliance Focus:*

- Regular audits.
- Employee training for EHS standards.

# CONCLUSION

- LABS is a widely used, biodegradable surfactant with strong industrial relevance and scalability.
- The QuantiVEX assessment shows that environmental and health risks can be effectively managed through modern EHS practices.
- Sustainable production is achievable via zero liquid discharge, emission control, and green chemistry integration.
- Overall, LABS remains a safe, efficient, and eco-friendly choice for detergent applications.

# REFERENCES

[https://drive.google.com/drive/folders/1M1Y2FUPDgXaKLrmNC5p3h05mdkfcBPKD?usp=drive\\_link](https://drive.google.com/drive/folders/1M1Y2FUPDgXaKLrmNC5p3h05mdkfcBPKD?usp=drive_link)

# THANK YOU