QuantiVEX

Quantifying Chemistry. Qualifying Tomorrow.

Business Presentation

TEAM

QUANTIVEX
(CEO : Nithin T M)

R&D
- Pulkit
- Aditya
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MARKET
- Sajag
- Shivam
- Venugopal
- Priyanka

TECHNICAL
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- Arnav
- Om Singh

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: $R{-}COO{-}(CH_2CH_2O)_n{-}R'$
R: Fatty acid chain (C_{12}–C_{18})
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   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: 120–150ºC, ~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):
- $C_{12}H_{24}O_2 + C_3H_7NO_2 \quad C_{15}H_{29}NO_3 + H_2O$
- Base/enzyme catalysis
- Water removed via evaporation
- **Neutralization:**
- $C_{15}H_{29}NO_3 + NaOH \quad C_{15}H_{28}NNaO_3 + H_2O$
- 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:
2. $C_{12}H_{24}O_2 + SOCl_2 \quad C_{12}H_{23}ClO + SO_2 + HCl$
    - Toxic byproducts   gas scrubbing needed
3. Amidation with Sarcosine:
4. $C_{12}H_{23}ClO + C_3H_7NO_2 \quad C_{15}H_{29}NO_3 + HCl$
5. Neutralization:
6. $C_{15}H_{29}NO_3 + NaOH \quad C_{15}H_{28}NNaO_3 + H_2O$

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: $R{-}C_6H_4{-}SO_3Na$
R: Linear alkyl chain ($C_{10}{-}C_{14}$)
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 / $AlCl_3$ / Zeolite
Selectivity for 2-phenyl isomer preferred for biodegradability
Sulfonation:
LAB + SO_3 LAB Sulfonic Acid
Continuous film reactor or falling film sulfonator
Controlled to avoid disulfonation
Neutralization:
LABSA + NaOH   LABS (sodium salt) + H_2O

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_3 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

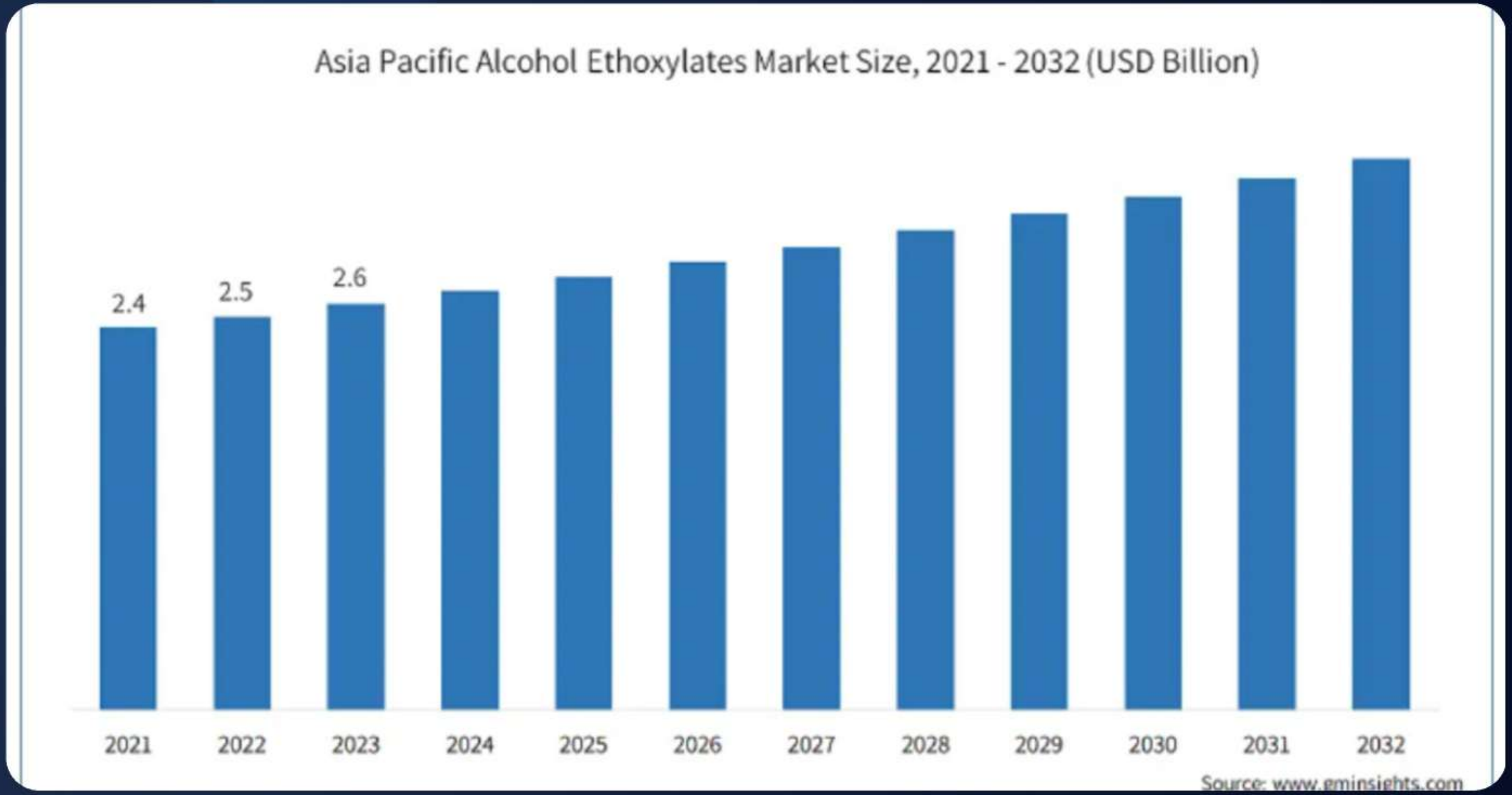
FAE

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.

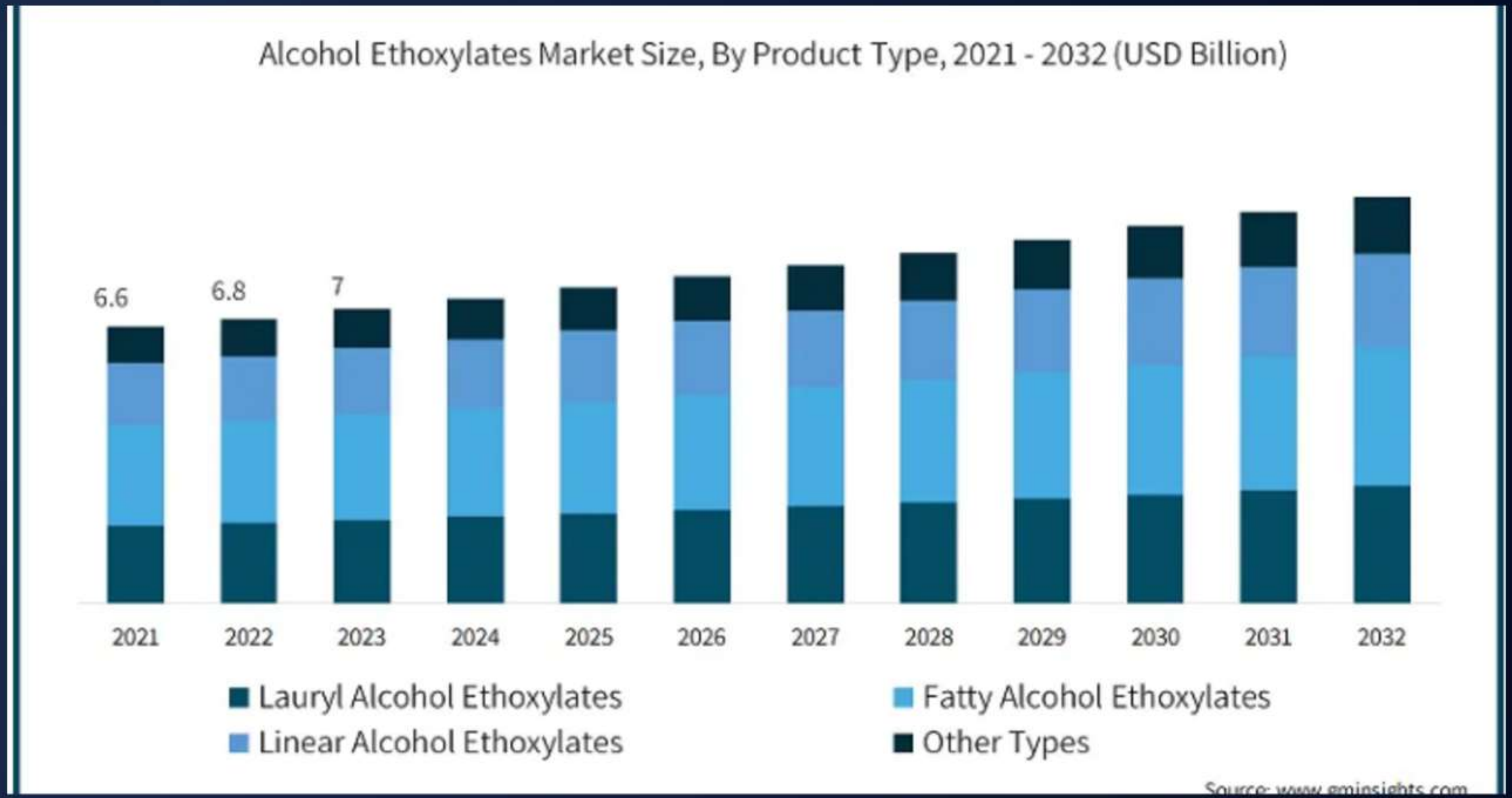
- *Production Hotspots:*
  - *Asia-Pacific (China, India dominate production)*
  - *Europe & North America (tech innovation focus)*



FAE

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) ×100 =* ***40.9%***
- *ROI : 22.3%, payback period : 4.5 years*



LABS

LABS - Market Overview

- *Definition: Anionic surfactant in detergents and household cleaning*

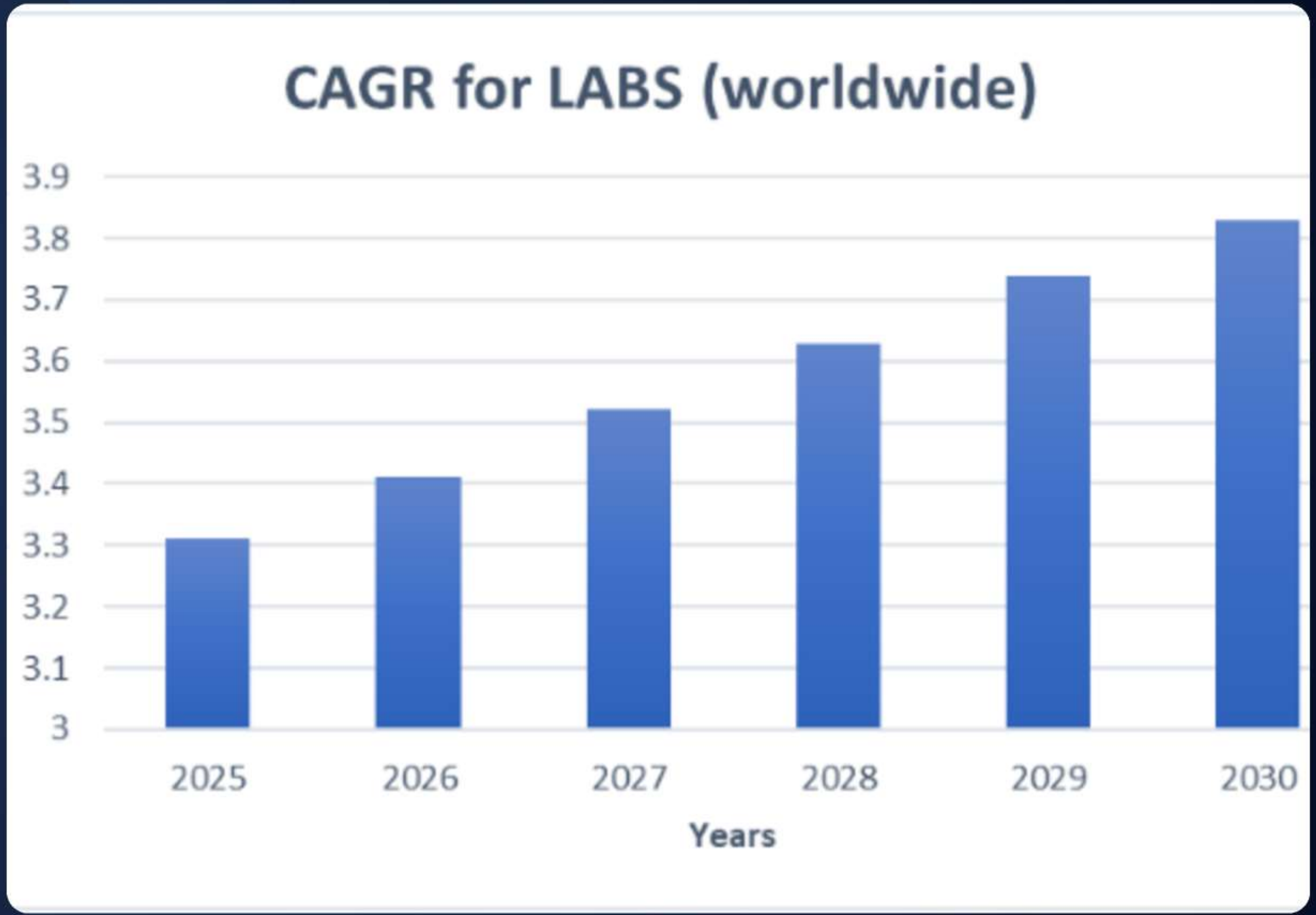
- *Market Size (2023): ~$10.1 billion*
- *Expected CAGR (2024–2029): ~3.8%*

- *Applications: Laundry, dishwashing liquids, industrial cleaners, Leather industry, Paper industry*

LABS

LABS - Production & Demand

- *Raw Inputs: LAB (from kerosene), SO_3*
- *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) × 100 = **49.62%***
- *ROI of 16.5%, payback period of 6 years*



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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:

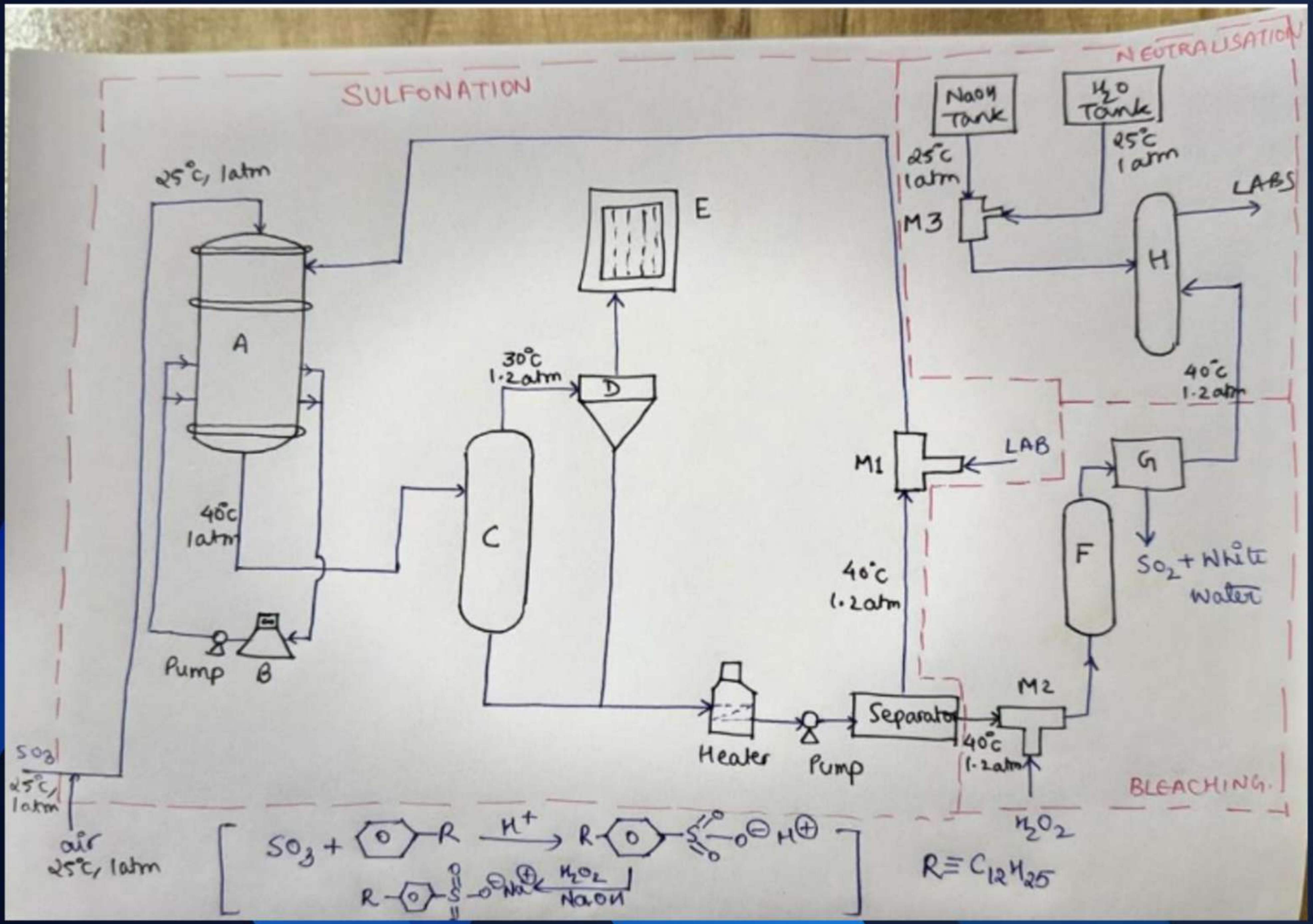
Name	Annual Export Value (in millions USD)	Key Destinations	Quantity (MT/year)
Nirma Ltd.	80 - 100	Vietnam, UAE, Egypt ,Brazil, South Africa	60,000 - 80,000
Tamilnadu Petroproducts Ltd	50 -70	Turkey, Indonesia, Nigeria, Iraq	40,000 - 60,000
Re Reliance Industries Ltd.	30 - 50	Bangladesh, Sri Lanka, kenya, 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	-
Total	**42.35**	**42.38**

Table 3: Summary of Mass Flow Rates in the Reactor

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3.2 Bleaching

Reaction:
LABSA (dark coloured) + $H_2O_2 \longrightarrow$ 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.

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

LABS

Energy Requirements:

4.4 Overall Balance

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

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

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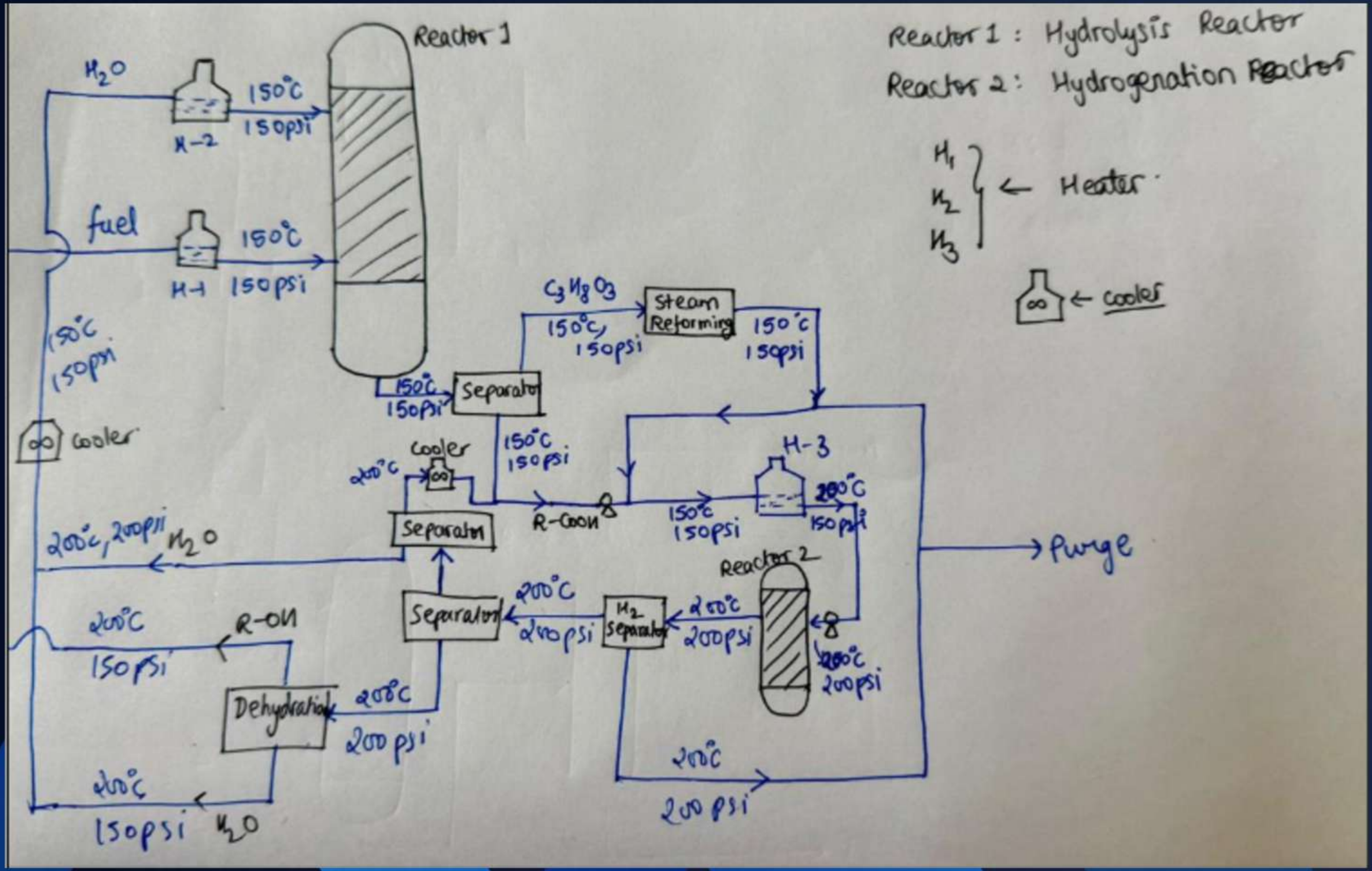
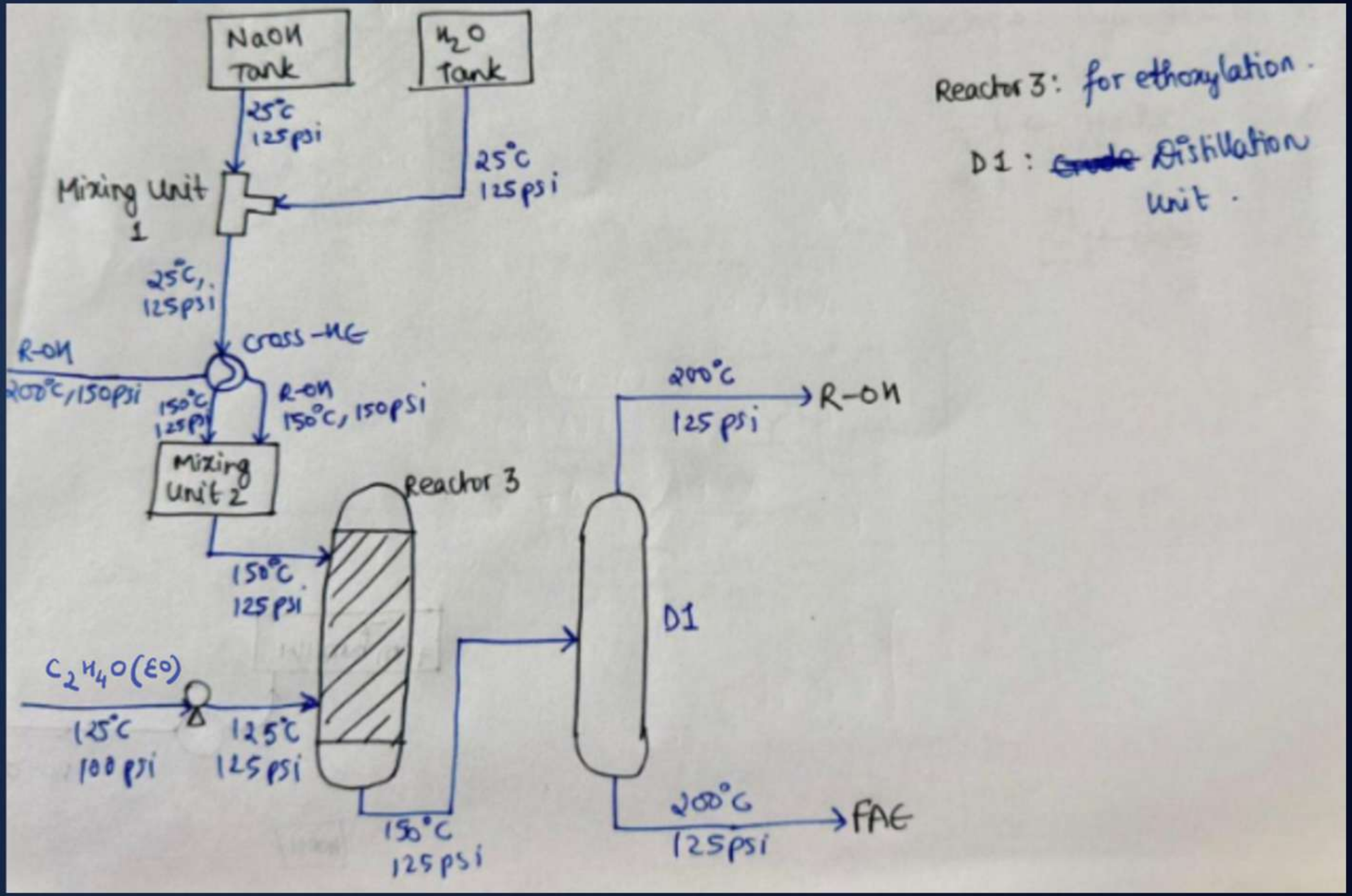
Process FlowSheet





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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
Total	**30.26**	**30.26**

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
Total	**4.44**	**4.44**

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
Total	**26.3**	**26.4**

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
Total	**26.93**	**26.93**

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
Total	**46.03**	**46.03**

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:

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

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

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^3	Scrubbing & Adsorption
VOCs	<10 ppm	Adsorption on Activated Carbon

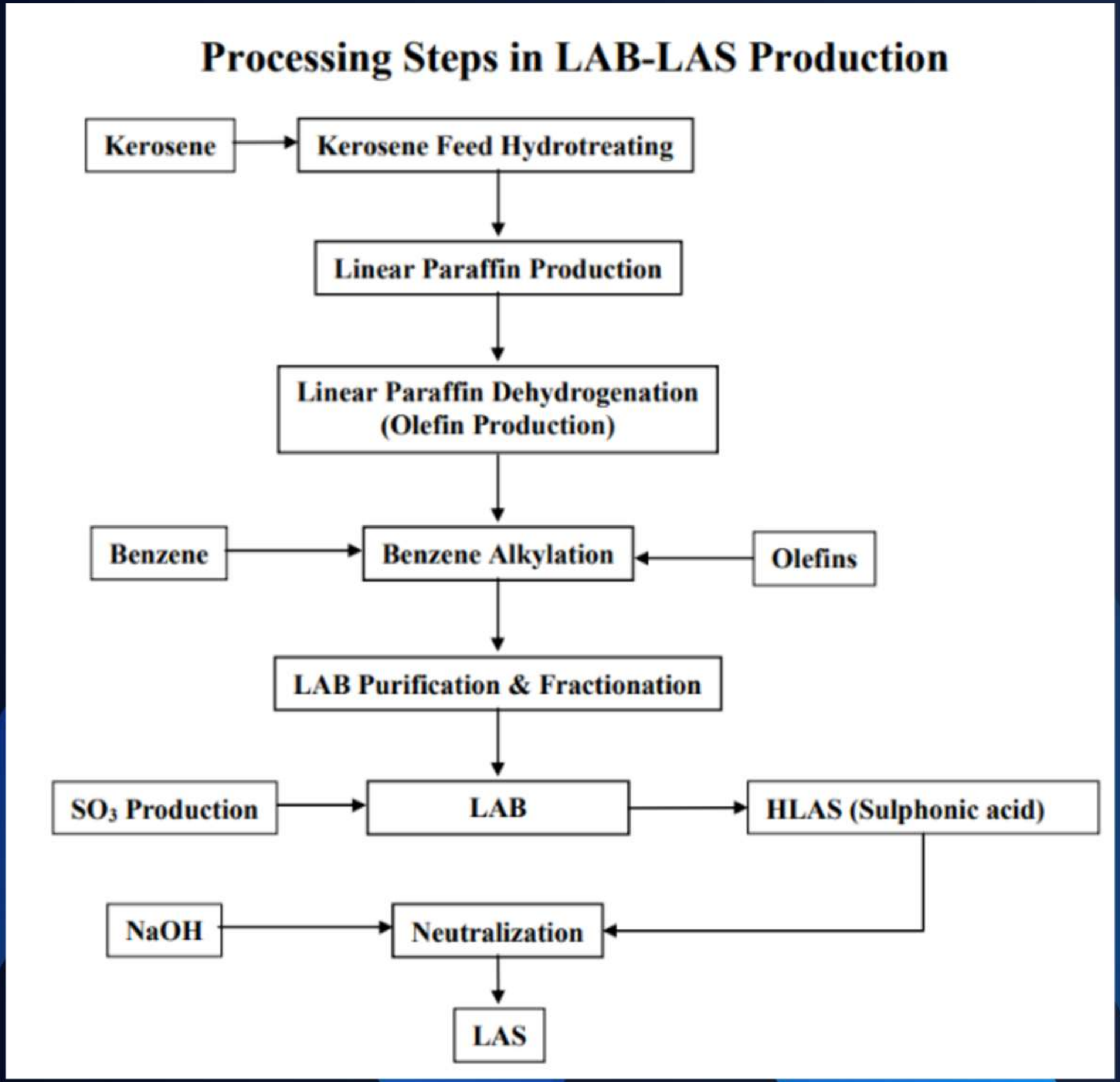
LABS

WASTE TREATMENT AND ZERO LIQUID DISCHARGE (ZLD):

- *Acid Recovery*: H_2SO_4 neutralized with $NaOH/Ca(OH)_2$ $Na_2SO_4/CaSO_4$ 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 NH_3.
  >VOCs: Removed using activated carbon & biofiltration.

LABS

PROCESSING STEPS



Occupational Exposure Limits (OELs)

Chemical	TWA(8hr)	STEL(15min)	Health Risks
Sulfuric Acid (H_2SO_4)	1 mg/m^3	3 mg/m^3	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:
  >H_2SO_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

THANK YOU