CHEMEVERSE

TEAM STRUCTURE

MANAGEMENT

Anshika Agrawal
(CEO)

MARKET ANALYSIS

GENERAL MANAGERS

1. Kshitij Srivastava
2. Rounak Mishra
3. Krish Agarwal
4. Tushar Jain

R & D

PRINCIPLE SCIENTISTS

1. Kamal Jaiswal
2. Vibhanshu
3. Sahil Kumar
4. Manas Todi

TECHNICAL SERVICES

PRINCIPLE DESIGN ENGINEERS

1. Tanvi Manhas
2. Harshvardhan Agarwal
3. Pratyush Biswal
4. Armaan Pratik Pasayat

EHS

SUSTAINABILITY OFFICERS

1. Om Singh
2. Yash Upadhyay
3. Arsh Jaswal
4. Amish Verma

RESEARCH AND DEVELOPEMENT

Screened 3 Specialty Chemicals:

- Cypermethrin (Agrochemical)
- SLES (Surfactant)
- PCE (Polymer for construction additives)

Designed Lab-Scale Synthesis Routes:

- Based on patents and literature review

Cypermethrin:

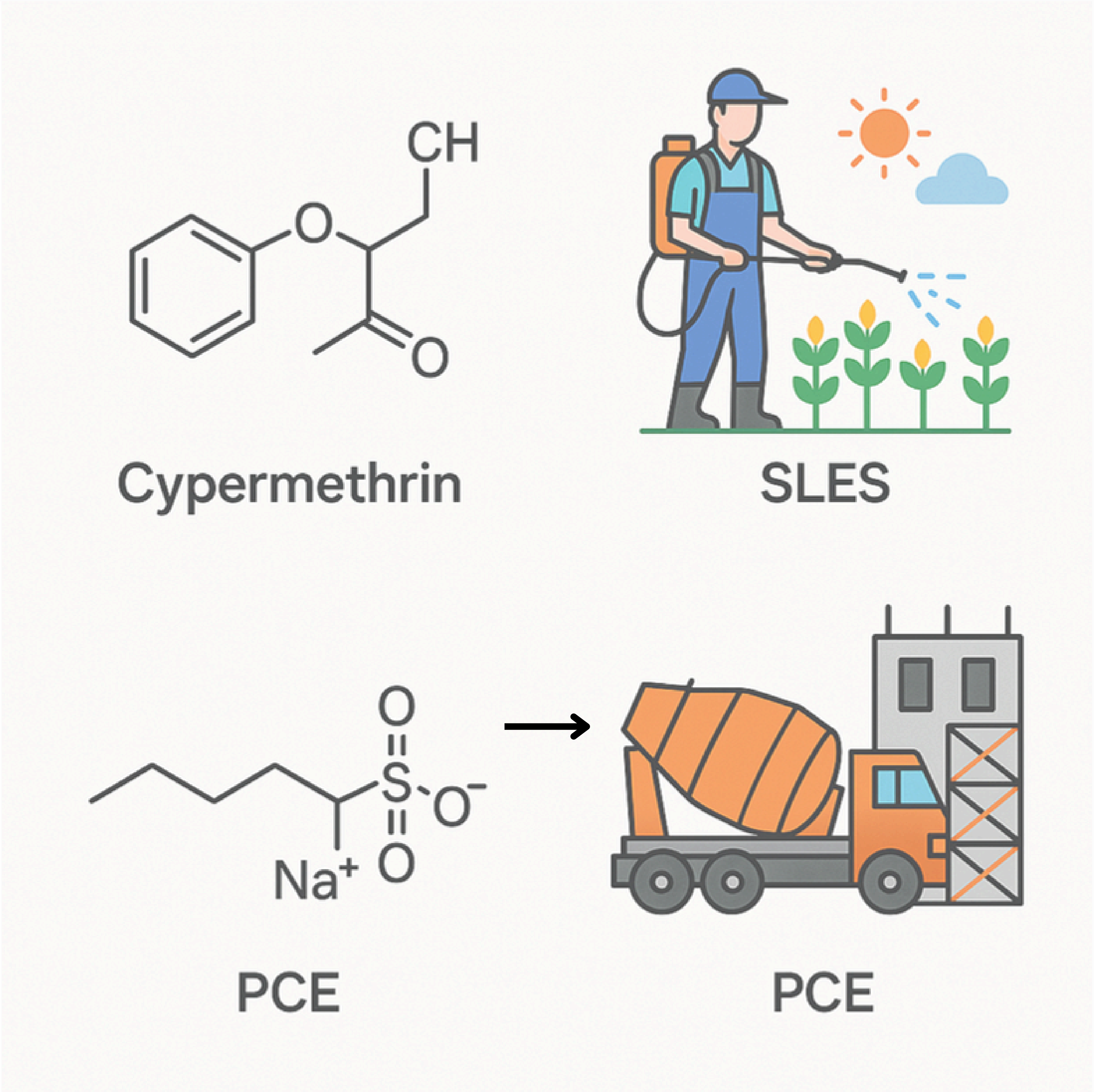
- Proposed a 2-step synthesis
- Achieved high yield (98.8%), better purity, and shorter reaction time

SLES:

- Analyzed 3 synthesis methods:
- SO_3 process, Ziegler, and OXO routes
- Compared to yield, feasibility & scalability

PCE:

- Developed a 2-step process: copolymerization + side-chain attachment
- Achieved ~85–90% purity
- Included green alternatives using bio-based PEGs



RESEARCH AND DEVELOPMENT

CRITERIA	CYPERMETHRIN	SLES	PCE
APPLICATION SECTOR	Pesticides/Agriculture	Personal Care/ FMCG	Construction / Infrastructure
MARKET ANALYSIS	High seasonal demand	High, stable demand	Rapidly growing, high-value
IMPORT DEPENDENCY	Moderate	High	High
PROFIT MARGIN POTENTIAL	Moderate	Moderate	High
GREEN CHEMISTRY POTENTIAL	Moderate	Low (SO_3 / EO use)	High (bio-based, PEGs)
PURITY ACHIEVABLE	> 98.5%	~ 70 wt%	~ 85-90% with ultrafiltration
ENVIRONMENTAL IMPACT	Cyanide use, toxic intermediates	SO3, chlorinated by products	Minimal; cleaner process routes

MARKET ANALYSIS

Parameter	PCE (Polycarboxylate Ether)	SLES (Sodium Laureth Sulfate)
Primary Use	Superplasticizer in concrete	Surfactant in personal care & herbicides
Market Demand (India)	Very High – construction boom	High – FMCG & agro industries
Import Value (India)	$26.6 million	$342,803
Major Exporting Country	China (71.82%)	India (66.03%), Malaysia
Average Import Price (USD/kg)	$1.47	$1.27
Raw Material Cost (₹/kg)	₹94.57	₹148.56
Selling Price (₹/kg)	₹560	₹330
Profit Margin (₹/kg)	₹465.43	₹181.44
Environmental Factor	Green routes, bio-based options	Involves SO_3/EO handling
Chosen as Final Product?	✅ Yes	❌ No

TECHNICAL SERVICES

POLYCARBOXYLATE ETHER

- Developed a complete process for producing Polycarboxylate Ether, including material and energy balances, equipment sizing, and cost estimation.
- Included a clear scale-up strategy for industrial-level implementation.

SODIUM LAURETH SULFATE

- Designed a process to produce Sodium Laureth Sulfate, detailing reaction steps, material transformations, and heat management.
- Sized and selected suitable equipment, estimated costs, and planned for industrial-scale production.

ENVIRONMENT, HEALTH AND SUSTAINABILITY

- Identified key chemical wastes and their environmental impacts.
- Ensured regulatory compliance with COD, BOD, pH, TWA, and STEL limits.
- Designed a Zero Liquid Discharge (ZLD) system with recovery and reuse.
- Outlined safety protocols for handling and storage.
- Developed recovery methods for ethanol, acids, CMP, and MPEG.

Polycarboxylate Ether (PCE)

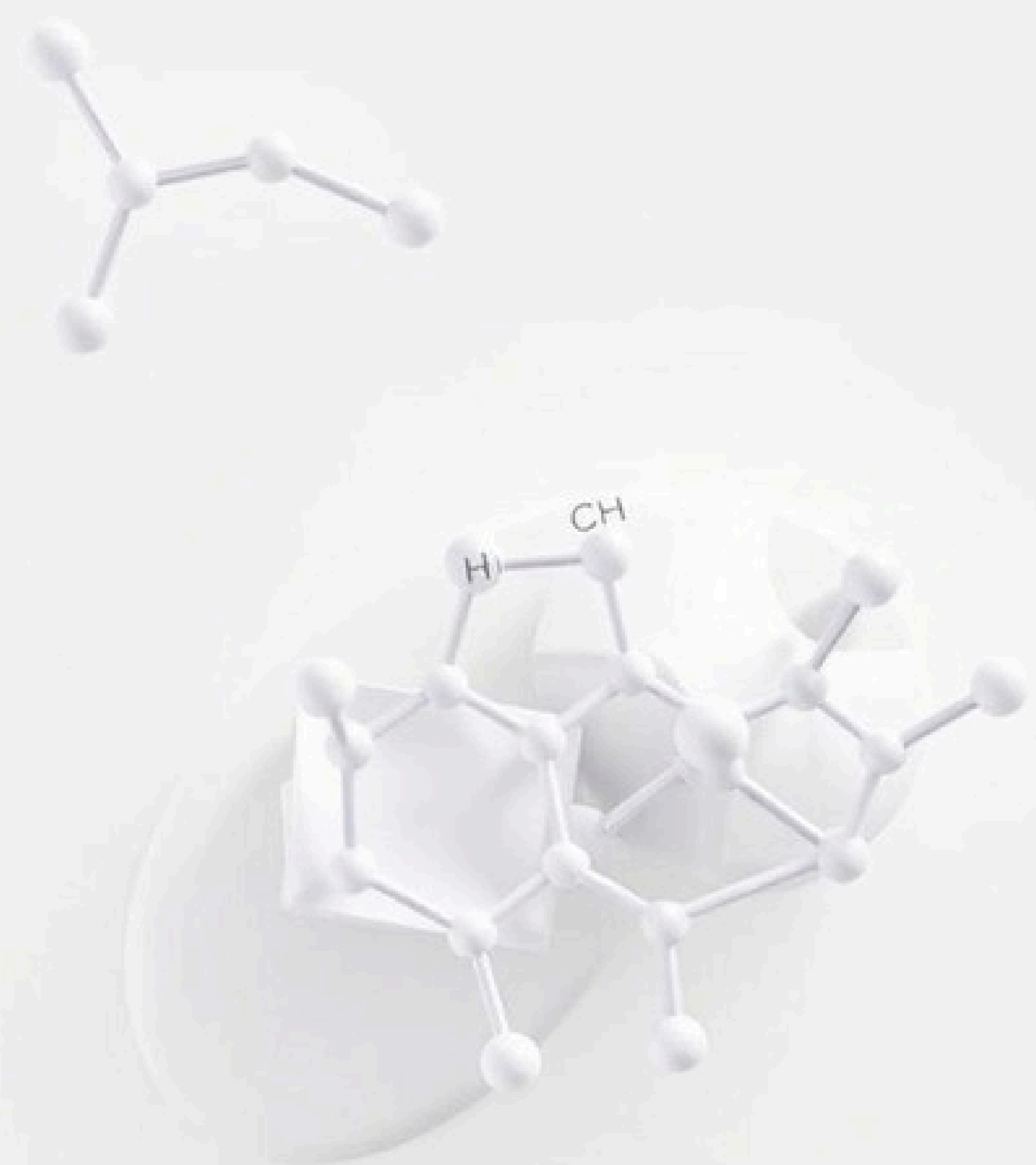
$CH_2=C(R)-COO-(CH_2CH_2O)_nR'$

- "PCE was selected because it sits at the intersection of market need, economic viability, technical feasibility, and environmental sustainability."
- R&D developed a lab-scale synthesis with up to 90% yield and ~85–90% purity
- Technical Services scaled this to a 1000 kg/day plant with material balance and capital cost estimation
- EHS designed a low-impact waste management plan based on green synthesis options

- Total Raw Material Cost: ₹94.57 per kg
- Selling Price: ₹560 per kg
- Profit per kg: ₹465.43

- India’s annual PCE imports: Over $26.5 million, mostly from China
- Strong import substitution potential

MARKET ANALYSIS



Polycarboxylate Ether (PCE)

Uses:

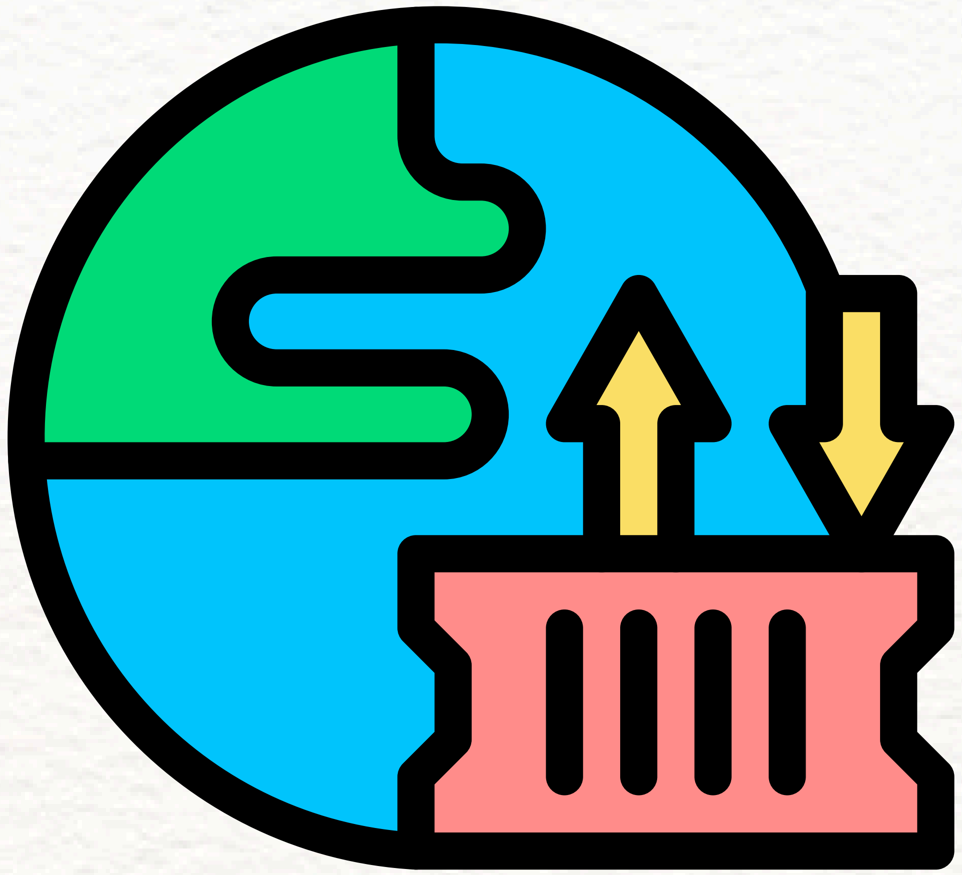
- Polycarboxylates are used as builders in **detergents**.
- Their high chelating power, even at low concentrations, reduces deposits on the laundry and inhibits the crystal growth of calcite.
- Polycarboxylate ethers (PCE) are used as **superplasticizers** in **concrete production**.

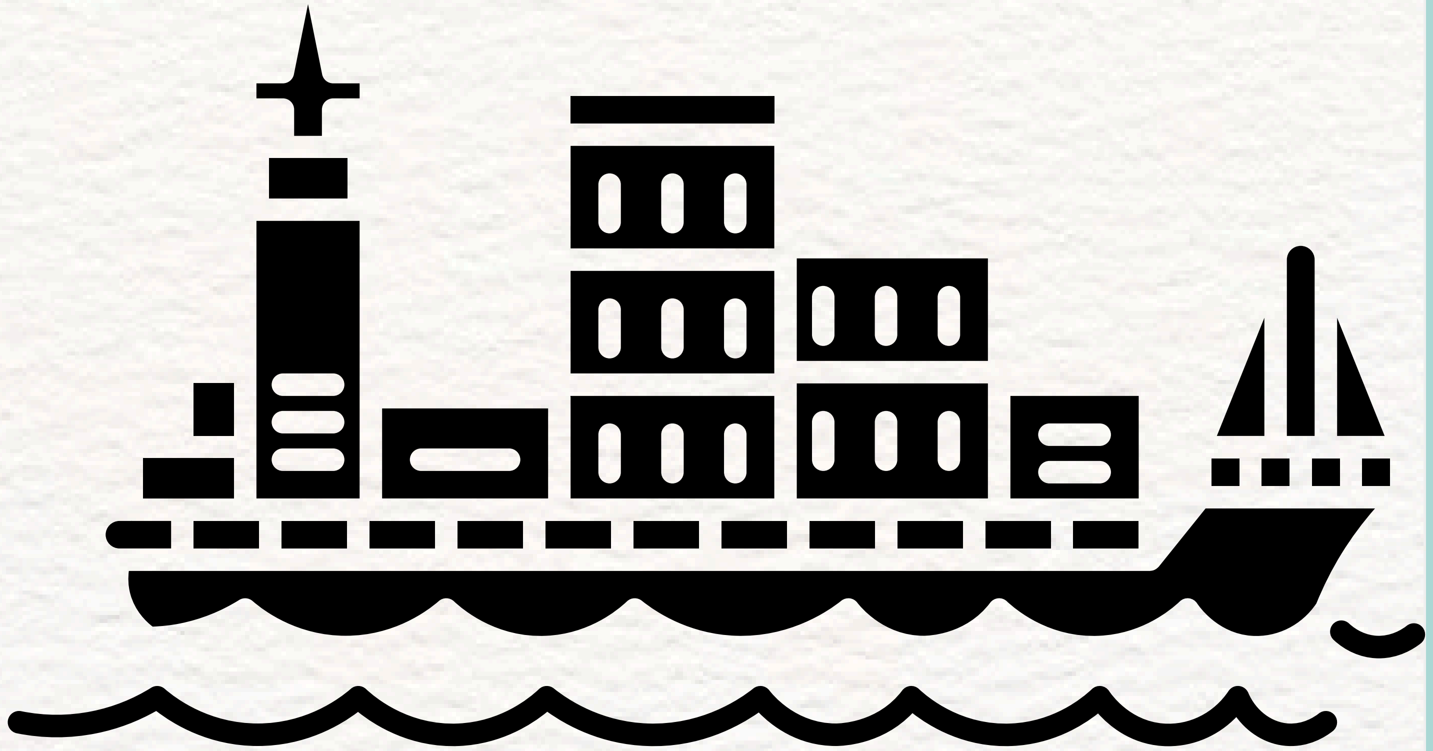
Alternatives:

1)Naphthalene Sulfonate Formaldehyde (SNF)
2)Melamine-based Superplasticizers (SMF)
3)Lignosulfonates
4)Polyacrylic Acid (PAA) & Polyvinyl Alcohol (PVA) based Superplasticizers

Advantages over Alternatives

- PCE has **higher water reduction capacity**, leading to higher strength and durability.
- PCE keeps concrete **flowable for 2-3 hours**, perfect for ready-mix concrete (RMC) and self-compacting concrete (SCC).
- PCE works effectively at 0.1-0.3% by weight of cement hence **cost effective** for longer runs.
- PCE uses steric hindrance and electrostatic repulsion to disperse cement particles evenly, reducing clumping & air bubbles.



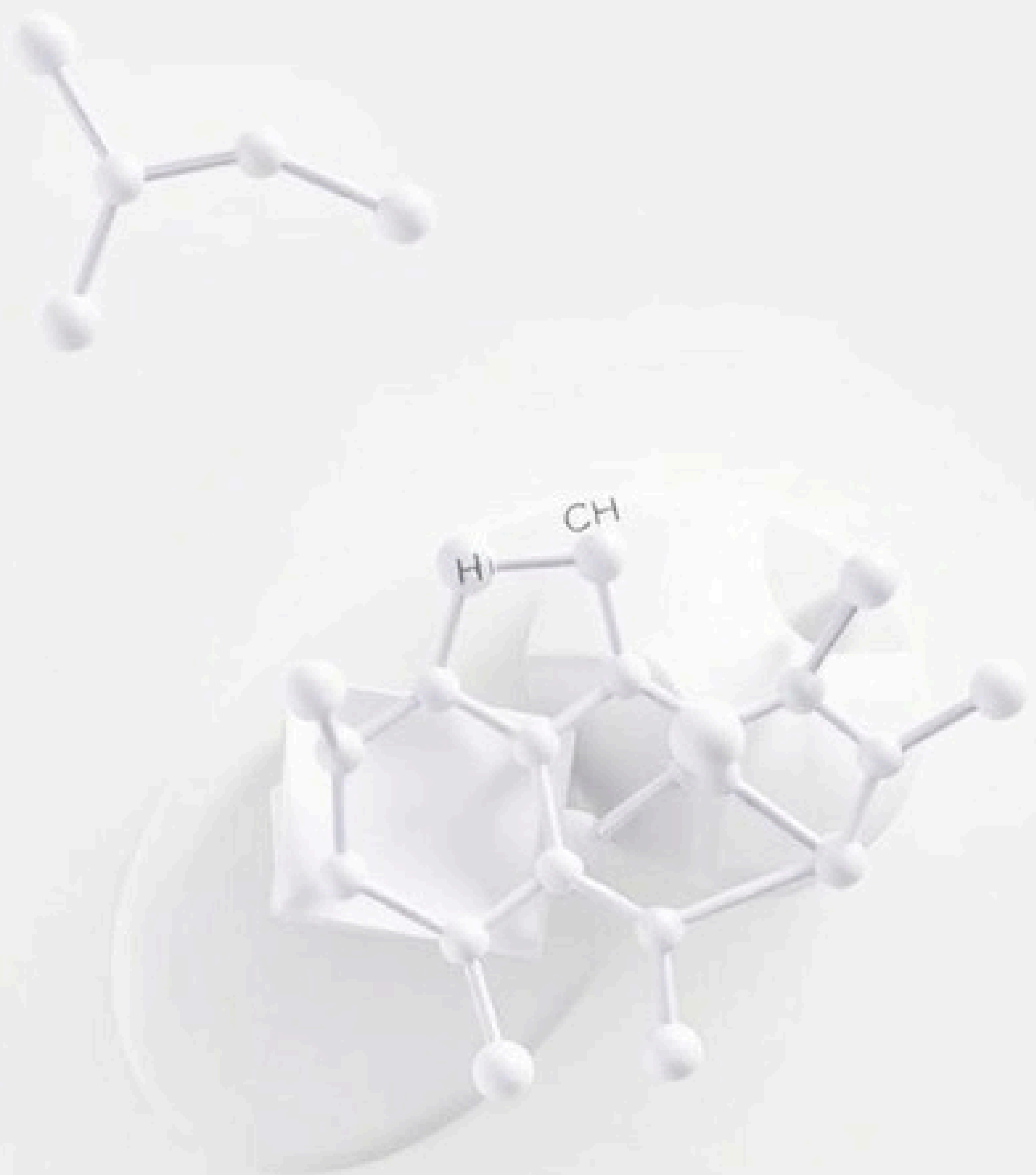


Magnitude of imports in India

- Polycarboxylate Ether worth $26,587,962 has been imported.
- Average import price for polycarboxylate ether was $1.47.
- China was the largest exporter of polycarboxylate ether accounting for 71.82% of the total imports of polycarboxylate ether.
- The month of Apr 2016 accounted for the highest number of import shipments.

Economic feasibility:

- Input Raw Materials with cost:
  - Acrylic acid - 350 g at 100 rupees per kg costs 35 rupees
  - Methoxy Poly Ethylene Glycol - 350 g at 110 rupees per kg costs 38.5 rupees
  - Potassium Carbonate - 15 g at 90 rupees per kg costs 1.35 rupees
  - Ethanol - 85 rupees per litre => 108 rupees per kg (density = 789 kg/m3) => 30g costs 3.24 rupees
  - Azobisisobutyronitrile(AIBN) - 2 g at 950 rupees per kg costs 1.9 rupees
  - 3-Chloro-2-methyl-1-propene (CMP) - 30 g at 100 rupees per kg costs 3 rupees
  - Methacrylic Acid - 80 g at 130 rupees per kg costs 10.4 rupees
  - Sodium Hydroxide - 15 g at 36 rupees per kg costs 0.54 rupees
  - Deionized water - (5 rupees per litre => 5 rupees per kg) 128 g at 5 rupees per kg costs 0.64 rupees
- Total Raw Material Cost: ₹94.57 per kg
- Selling Price: ₹560 per kg
- Profit per kg: ₹465.43



Sodium Laureth-2 Sulfate

Uses:

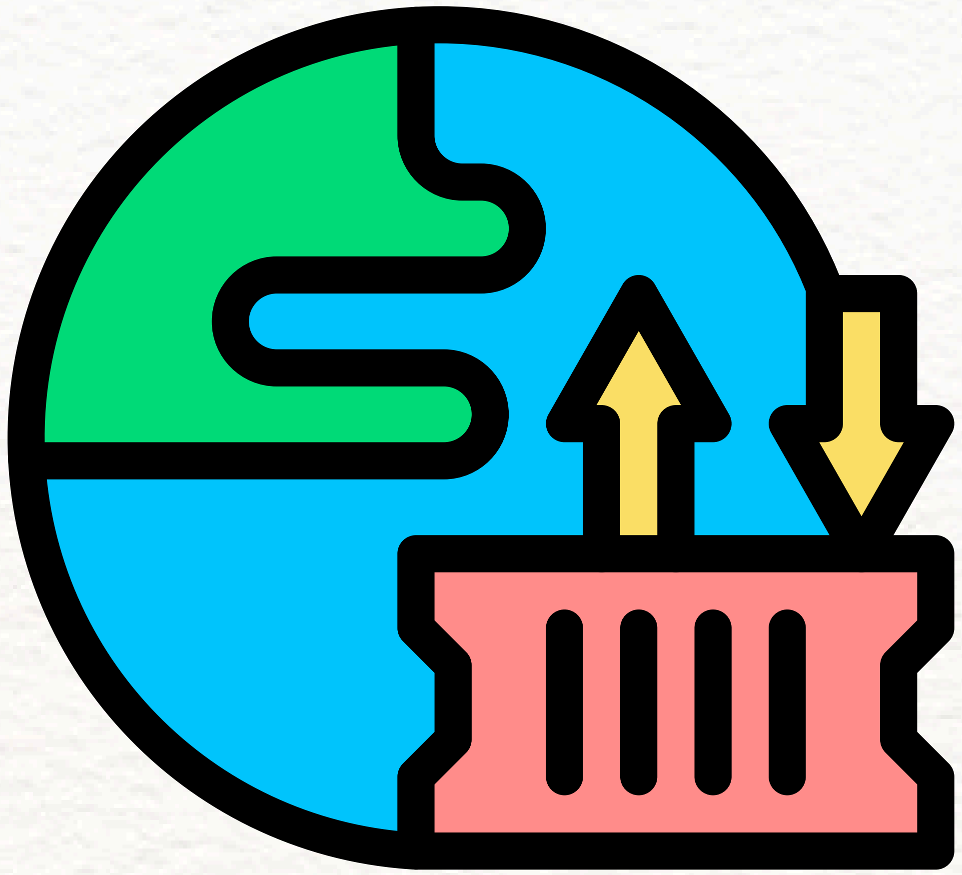
- SLES is used in many cosmetic products for their cleaning and emulsifying properties
- SLES in herbicides, is used as a surfactant to improve absorption of the herbicidal chemicals and reduces time the product takes to be rainfast, when enough of the herbicidal agent will be absorbed.

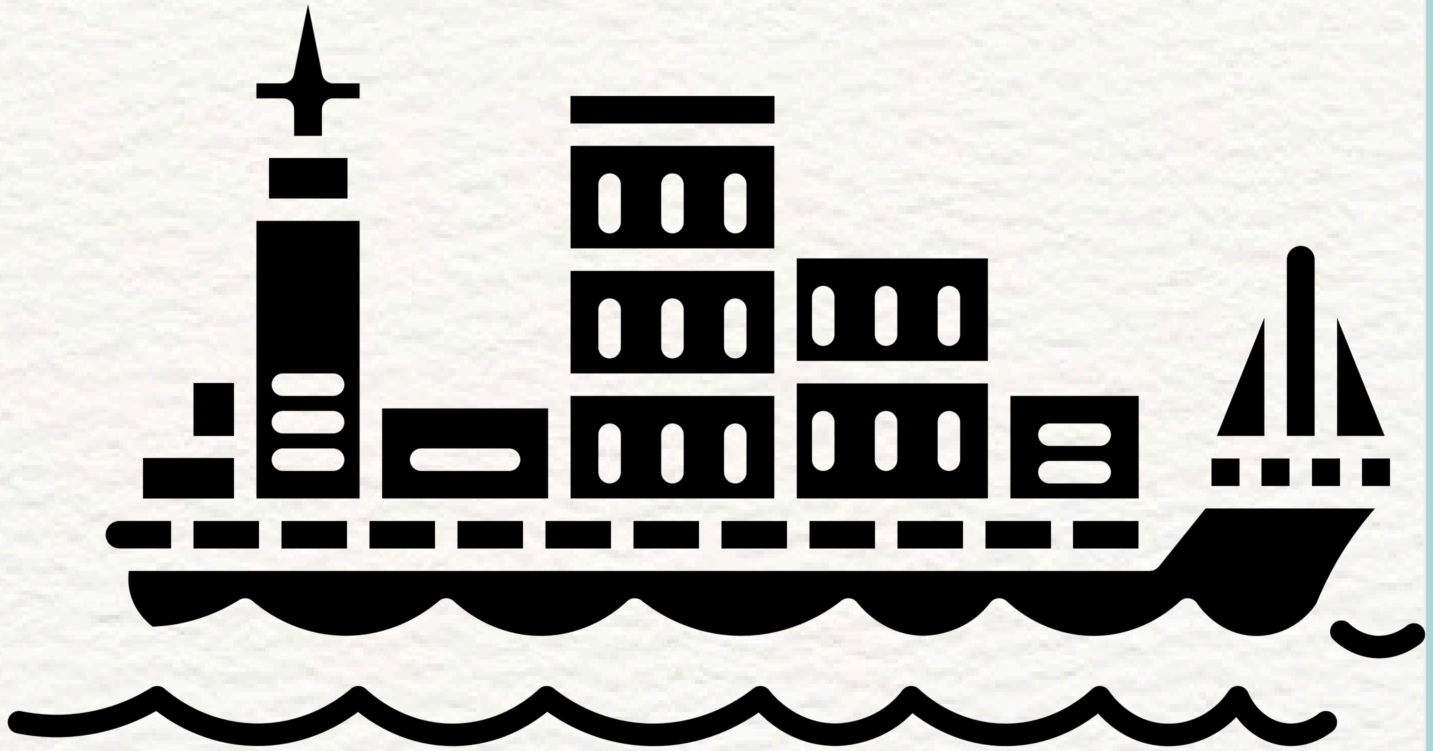
Alternatives:

1)Sodium lauroyl sarcosinate
2)Sodium dodecyl sulfate
3)Sodium myreth sulfate
4)Sodium pareth sulfate

Advantages over Alternatives

- SLES **produces richer and more stable foam**, making it more effective in cleansing and personal care applications.
- SLES is **milder on the skin and eyes** compared to Sodium Dodecyl Sulfate (SLS), which is known to cause stronger irritation.
- SLES is more widely produced and cheaper than Sodium Myreth Sulfate, making it the preferred choice in mass-market products.
- SLES **has a better biodegradation rate,** reducing its long-term environmental persistence compared to Sodium Pareth Sulfate.





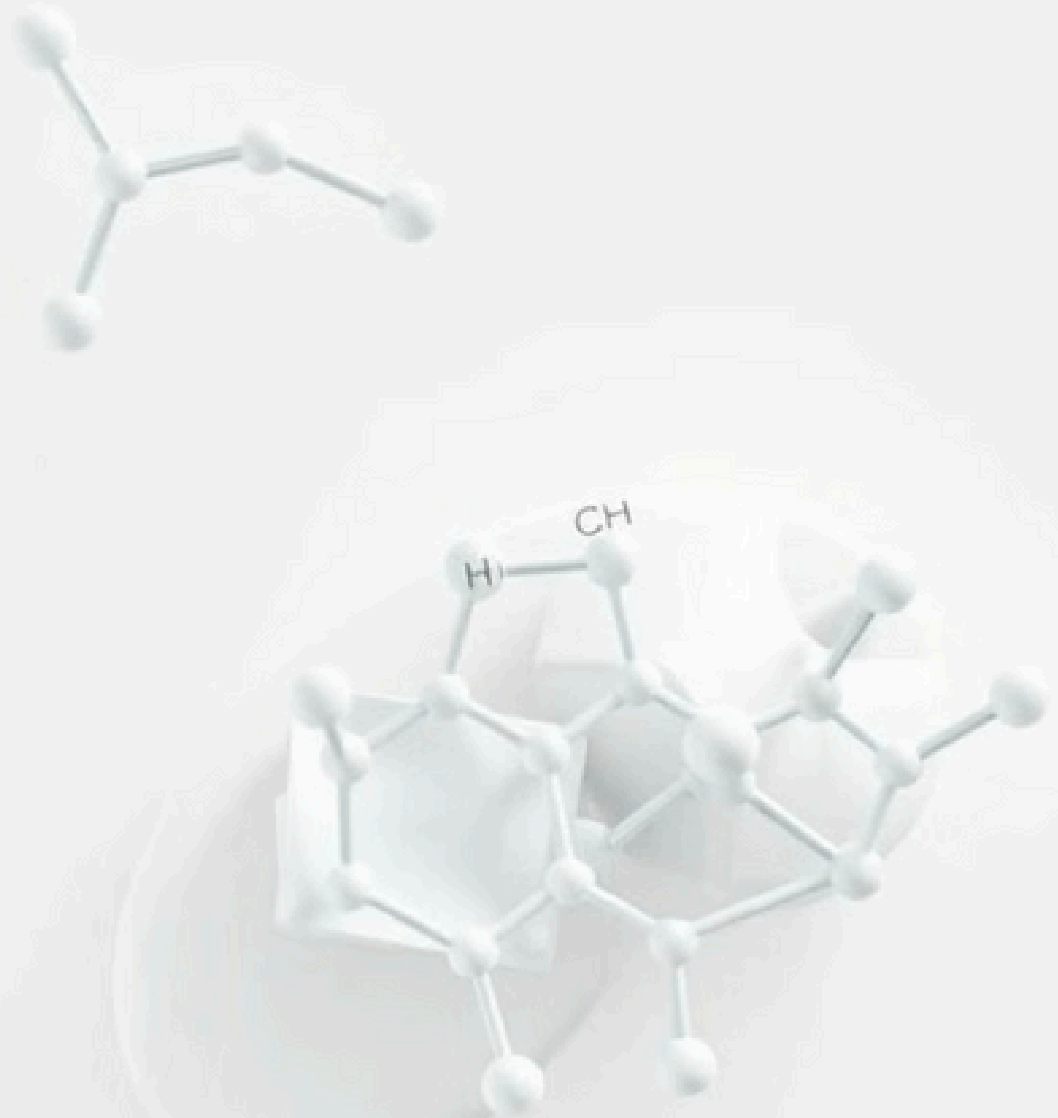
Magnitude of imports in India

- Sodium Lauryl Ether Sulphate worth $342,803 has been imported.
- Average import price for sodium lauryl ether sulphate was $1.27.
- Sodium Lauryl Ether Sulphate were imported from 6 countries
- India was the largest exporter of sodium lauryl ether sulphate accounting for 66.03% of the total imports of sodium lauryl ether sulphate
- Malaysia was the second largest exporter of sodium lauryl ether sulphate accounting for 16.32% of the total imports of sodium lauryl ether sulphate
- The month of Jan 2014 accounted for highest number of import shipments.

Economic feasibility:

- Input Raw Materials:
  - Dodecyl Alcohol ($C_{12}H_{26}O$) or Fatty Alcohol Ethoxylate ($C_{12}H_{25}(OCH_2CH_2)_nOH$)
  - Ethylene Oxide (C_2H_4O)
  - Sulfur Trioxide (SO_3) or Chlorosulfonic Acid (HSO_3Cl)
  - Sodium Hydroxide Solution (NaOH, ~50 wt%)
- Raw Material Costs:
  - Dodecyl Alcohol ($C_{12}H_{26}O$): 510.6 g at ₹205/kg = ₹104.673
  - Ethylene Oxide (C_2H_4O): 241.5 g at ₹75/kg = ₹18.1125
  - Sulfur Trioxide (SO_3): 219.4 g at ₹75/kg = ₹16.455
  - Sodium Hydroxide (50% Solution): 219.2 g at ₹42.5/kg = ₹9.316
- Total Raw Material Cost: ₹148.56 per kg
- Selling Price: ₹330 per kg
- Profit per kg: ₹181.44

RESEARCH AND DEVELOPMENT



Sodium Laureth-2 Sulfate

Sodium Laureth-2 Sulfate (SLES) is an important anionic surfactant used in various personal care and cleaning products. This presentation explores its raw materials, manufacturing processes, and applications.

Raw Materials and Chemicals

- Dodecyl alcohol/Lauryl alcohol ($C_{12}H_{26}O$)
- Sulfur trioxide (SO_3)
- Ethylene oxide (C_2H_4O)
- Sodium hydroxide solution (NaOH, ~50 wt%)

Ethoxylation & Sulfation Method

- High purity(~70% by weight)
- flexible scale
- Each step gives high yields, reducing waste and making the process efficient
- The reactions occur under relatively moderate and controllable conditions

Ethoxylation Process

Primary Process

This step adds ethylene oxide units to the fatty alcohol, converting it into a fatty alcohol ethoxylate.

Purpose

- Improves the water solubility of the final product
- Increases mildness and foaming ability of SLES (vs. plain sulfated alcohols)
- Allows tailoring of product properties by adjusting the ethoxylation level (n)

Sulfation Process

Process Description

This step introduces a sulfate group to the ethoxylated alcohol, forming the acidic intermediate (ethoxysulfate).

Purpose

- Converts the nonionic ethoxylate into an anionic surfactant precursor
- Enables the molecule to exhibit detergency, foaming, and emulsifying properties
- Prepares the intermediate for neutralization into the final usable surfactant form

Neutralization and Scrubbing

Neutralization

Neutralizes the acidic sulfate ester intermediate using sodium hydroxide to form sodium lauryl ether sulfate (SLES).

Purpose:

- Produces the final anionic surfactant in stable salt form (SLES)
- Adjusts the pH to make it suitable for cosmetic and cleaning formulations
- Yields a safe, usable aqueous solution (~70 wt%) ready for application or formulation

Scrubbing

Removes and captures harmful gaseous by-products like SO_3 or HCl from the reaction off-gases.

Purpose:

- Prevents release of toxic gases to the environment
- Converts them into valuable or manageable by-products (e.g., ~33 wt% HCl)
- Ensures safety and regulatory compliance

Alternative Manufacturing Processes

Ziegler-Alfol Process

A specialized manufacturing route that produces high-quality fatty alcohols using organometallic catalysts.

OXO Process (Hydroformylation Route)

An industrial process that converts olefins to aldehydes and then to alcohols using synthesis gas.

Comparison of Manufacturing Methods

Method	Advantages	Disadvantages	Ideal Use
Ethoxylation & Sulfation	High purity, flexible scale	May require more specialized equipment	Personal care products Eco-friendly
Ziegler Process	Selective product, consistent quality	Requires specific catalysts	Eco-friendly and sustainable products
OXO Process	High throughput, versatile feedstocks	Possible impurities in the final product	Industrial applications with cost concerns

Applications and Benefits

Personal Care

Used in shampoos, body washes, and facial cleansers for its excellent foaming and cleansing properties

Household Cleaning

Effective in laundry detergents and dish soaps due to its detergency and emulsifying abilities

Eco-friendly Options

Modern manufacturing processes can be optimized for sustainability and reduced environmental impact

Industrial Applications

Utilized in various industrial cleaners and processes requiring effective surfactants

Cypermethrin

$C_{22}H_{19}Cl_2NO_3$

Synthesis Method

The present invention relates to an improved method for synthesizing cypermethrin, a widely used pyrethroid insecticide, ensuring high yield, purity, and efficiency.

Pyrethroid Insecticide

Cypermethrin belongs to the pyrethroid family of insecticides, which are synthetic compounds designed to control pest populations effectively.

Background of the Invention

Pyrethroid Family

Cypermethrin is a synthetic insecticide belonging to the pyrethroid family, used extensively for agricultural and household pest control.

Traditional Methods

Traditional synthesis methods involve multiple steps that are time-consuming and energy-intensive.

Improved Process

The present invention provides a more efficient synthesis process with improved reaction conditions, resulting in high-purity cypermethrin with minimal by-products.

Summary

Reaction

The invention provides a method for synthesizing cypermethrin by reacting 3-phenoxybenzaldehyde with sodium cyanide under controlled conditions to form cyanalcohol

Esterification

Followed by esterification with DV-acyl chloride to yield cypermethrin

Results

The process achieves high purity (>98.5%) and minimizes the presence of unreacted starting materials

A phase-transfer catalyst is used to enhance reaction efficiency and selectivity.

Detailed Description of the Invention

Materials Required:

- **Sodium cyanide (NaCN)**
- **3-phenoxybenzaldehyde**
- **DV-acyl chloride**
- **Phase-transfer catalyst**

  Diethylammonium ethanol-based ammonium chloride or benzyltriethylammonium chloride
- **Solvent**

  Normal hexane, suberane, toluene, or trichloromethane
- **Water**

Chemical Reactions

Formation of Cyanalcohol

3-Phenoxybenzaldehyde reacts with sodium cyanide in an aqueous medium:

$$C_6H_5OC_6H_4CHO + NaCN + H_2O \rightarrow C_6H_5OC_6H_4CH(OH)CN + NaOH$$

Esterification Reaction

The cyanalcohol undergoes esterification with DV-acyl chloride:

$$C_6H_5OC_6H_4CH(OH)CN + ClCOC_3H_6 \rightarrow C_6H_5OC_6H_4CH(COC_3H_6)CN + HCl$$

Reaction Process

Preparation of Reaction

Dissolve sodium cyanide (11–12 g) in water (60–70 g) and add phase-transfer catalyst (0.015 – 0.025 g) while stirring.

Formation of

Add 3-phenoxybenzaldehyde (36–39 g, 98.5% purity) to the mixture and stir at 25–35°C for 25–35 minutes to form cyanalcohol.

Addition of DV-acyl

Lower the temperature to 15–17°C, then add DV-acyl chloride (40–48 g, 98% purity).

Reaction Completion

Increase the temperature to 20 ± 3°C and maintain until cypermethrin concentration reaches ≥98.5%.

Separation and Purification

Stir for 8–12 minutes, allow the mixture to settle, and separate the waste water from the organic layer.

Final Product Isolation

Wash the upper organic layer with water twice, then remove the solvent under vacuum and negative pressure to obtain cypermethrin.

Advantages

1 hr

Reaction Time

Increased Efficiency: Shorter reaction time compared to traditional methods (7 hours)

98.5%

Product Purity

Higher Purity: Cypermethrin yield exceeds 98.5%, with minimal residual reactants

60%

Energy Savings

Optimized reaction conditions reduce solvent consumption and waste generation

Example Implementation

Preparation

Sodium cyanide (11.5 g) was dissolved in 65 g of water, with 0.02 g of phase-transfer catalyst added

Reaction

3-phenoxybenzaldehyde (37.5 g) and normal hexane (50 mL) were stirred at 25–30°C for 30 minutes

Completion

The reaction was completed at 20 ± 3°C, yielding 98.8% cypermethrin purity

Temperature Reduction

The temperature was reduced to 16°C, and 44 g of DV-acyl chloride was added

Final product yield: 99.5% after vacuum solvent removal.

This invention presents a highly effective and industrially scalable process for cypermethrin production, improving efficiency, cost-effectiveness, and product purity.

Polycarboxylate Ether (PCE)

Nature of the Invention

1

Chemical Formula

CH2=C(R)2COO2(CH2CH2O)nR2

- R: H or methyl
- R2: Alkyl or ether

2

Application

Superplasticizer for concrete

Key raw materials

- Acrylic Acid
- MPEG
- Potassium Carbonate
- Ethanol
- AIBN

Main Chain Formation

Copolymerization (Acrylic Acid, CMP, AIBN)

The main chain formation involves the copolymerization of acrylic acid with a chain transfer agent such as CMP (3-Mercaptopropionic acid), using AIBN (Azobisisobutyronitrile) as an initiator. This process forms the backbone of the PCE molecule.

Temp: 50-

70°C

Duration: 6-8 hrs

Reaction: n CH2=CHCOOH (Acrylic Acid) + m CMP + AIBN ^{3}

Poly(Acrylic Acid-co-CMP)

Side Chains Formation

Esterification with MPEG/PEGM Pendant carboxylic acid groups on the main chain are esterified with MPEG or PEGM to form side chains, creating a comb-like structure that enhances cement particle dispersion in concrete.

Reaction: Poly(Acrylic Acid-co-CMP) + n MPEG ^{3} PCE An acid catalyst typically promotes ester bond formation between the carboxylic acid groups of the main chain and the hydroxyl groups of MPEG/PEGM. Reaction conditions (temperature, time, catalyst concentration) are controlled to optimize esterification and PCE properties.

Neutralization

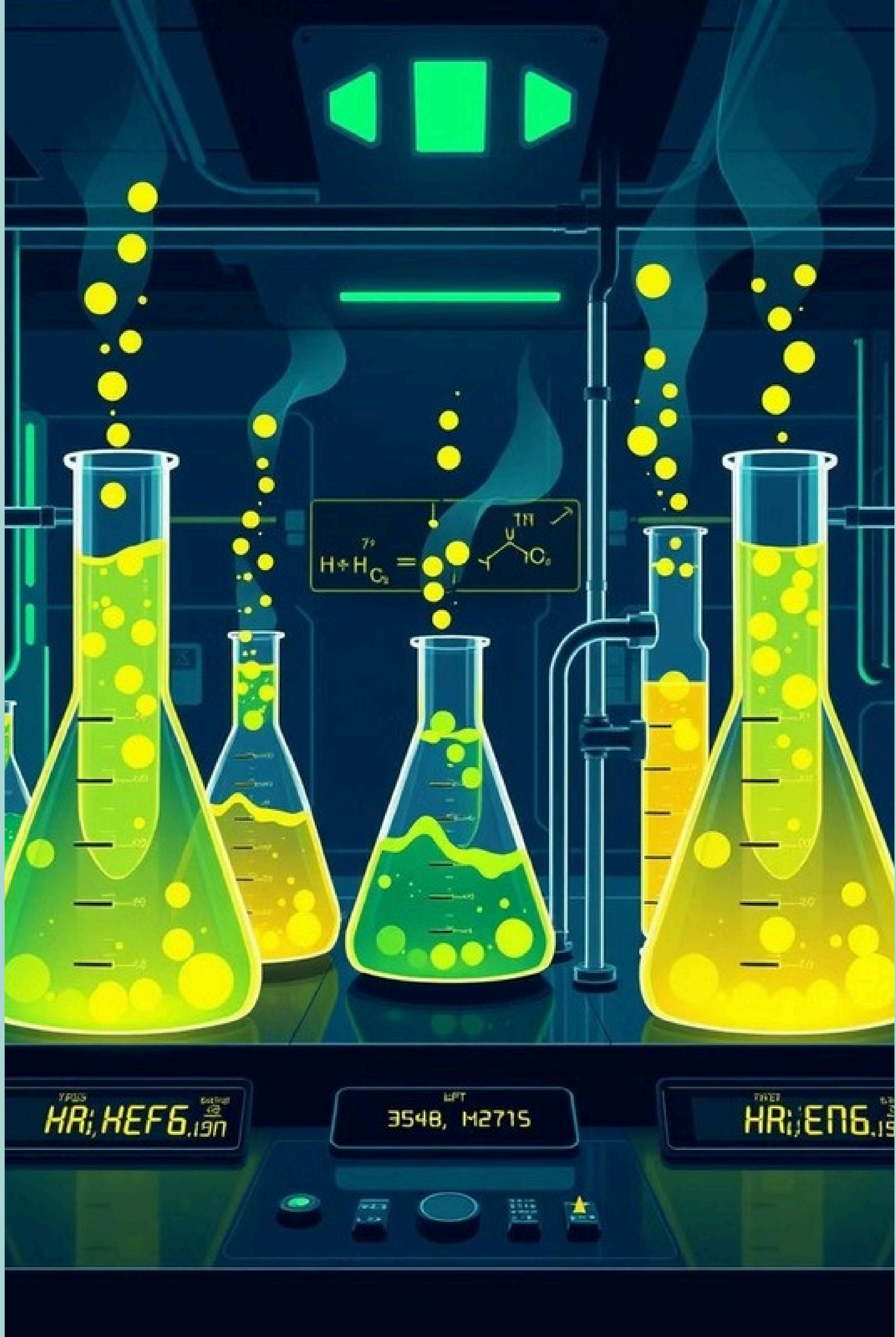
The reaction mixture is neutralized to a pH of 6-7 using sodium hydroxide (NaOH) or another suitable base. This step is crucial for ensuring the stability and optimal performance of the PCE product by converting the acidic carboxylic acid groups into their corresponding sodium salts.

Reaction: Poly(Acrylic Acid-co-CMP) + NaOH ^{3} Poly(Acrylic Acid-co-CMP)-

Na + H2O This neutralization process enhances the water solubility of the

PCE,

facilitating its effective dispersion in concrete mixtures and improving its superplasticizing capabilities. Proper pH control during neutralization is essential to prevent unwanted side reactions or degradation of the PCE polymer.



Purification Steps

Filtration

Remove Impurities

Solvent Evaporation

Concentration

Dialysis/Ultrafiltration

Purity Enhancement

Final Product Evaluation

1

Purity Testing

Gel Permeation Chromatography (GPC): Determines the molecular weight distribution and average molecular weight of the PCE polymer.

Fourier Transform Infrared Spectroscopy (FTIR): Identifies the presence of characteristic functional groups in the PCE structure to confirm the chemical composition.

2

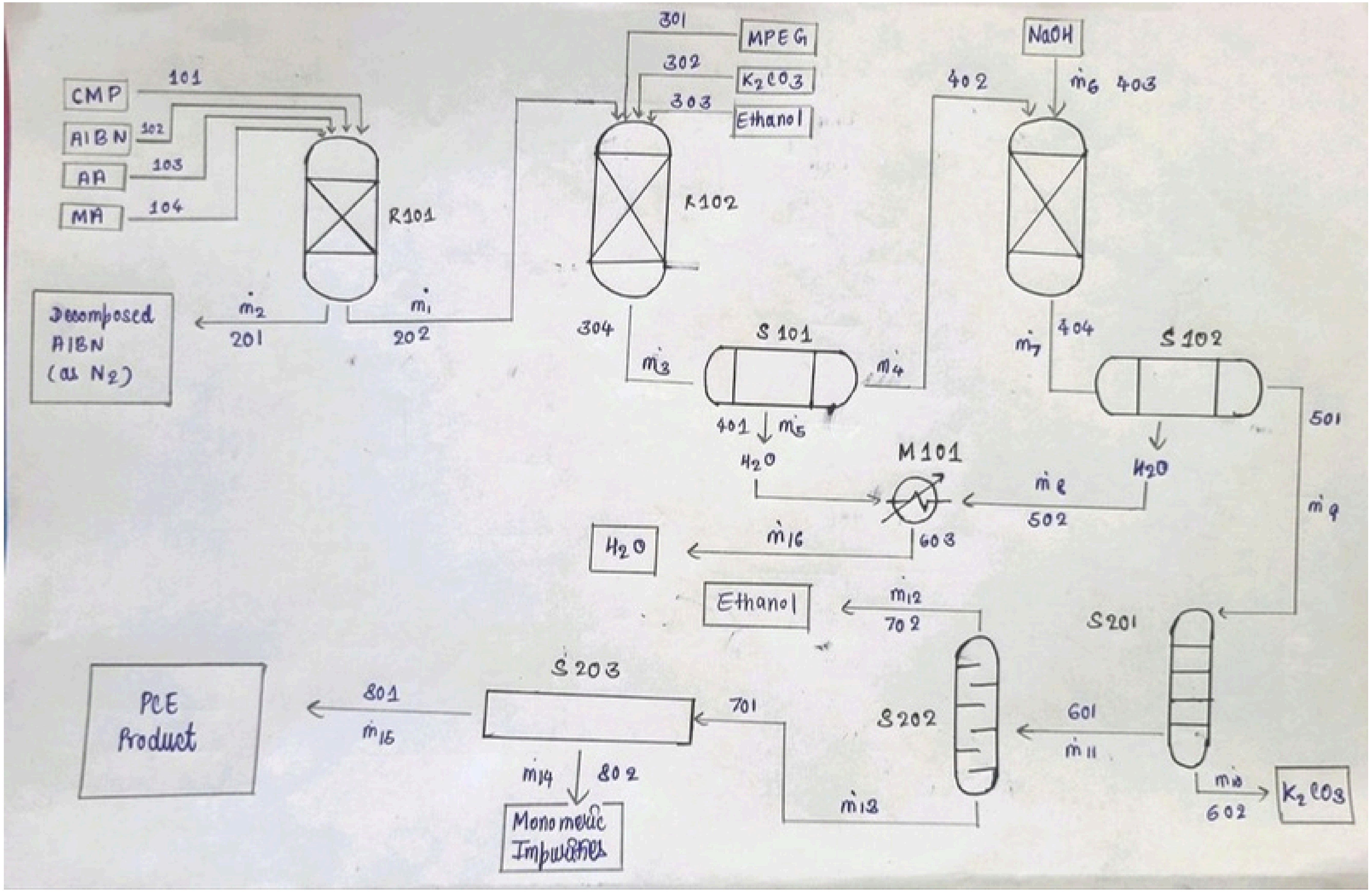
Yield

70%-90%

TECHNICAL SERVICES

PCE

PFD


CMP
AIBN
AA
MA
101
102
103
104
R101
Decomposed AIBN (as N2)
201
202
MPEG
K2CO3
Ethanol
301
302
303
304
R102
NaOH
402
403
R103
404
S101
401
H2O
S102
501
502
H2O
M101
603
H2O
Ethanol
702
S201
601
602
K2CO3
S202
701
S203
801
802
PCE Product
Monomeric Impurities

Reaction Process Conditions

R101 - Polymerization

Requires controlled temperature (around 70°C) and N_2 atmosphere to prevent oxidation. The synthesis temperature is critical for main chain formation.

R102 - Esterification

Requires controlled heating & continuous N_2 purge to remove byproduct water, ensuring efficient ester formation.

R103 - Neutralization

Requires pH control to ensure complete ionization of the polycarboxylate groups, typically around pH 6-7, for optimal reaction.

Separation and Purification Techniques

S101/S102 - Phase Separation

Decantation is used to separate immiscible liquids based on density differences.

S201 - Filtration

Solid-liquid filtration removes solid particles from the polymer solution.

S202 - Evaporation

Vacuum distillation is employed to remove volatile solvents from the polymer.

S203 - Purification

Membrane filtration is used to purify the polymer by removing impurities.

Process

We scaled up the lab synthesis to a plant producing 1000 kg/day

Input Materials :
AA - Acrylic Acid
CMP - 3-Chloro-2-methyl-1-propene
MA - Methacrylic Acid
AIBN - Azobisiso butyronitrile
MPEG - Methoxy Poly Ethylene Glycol
K2CO3
NaOH
Ethanol

Input Streams

Stream 101 : 11.864 kg/day CMP
Stream 102 : 0.05932 kg/day AIBN
Stream 103 : 35.502 kg/day AA
Stream 104 : 11.864 kg/day MA
Stream 301 : 118.64 kg/day MPEG
Stream 302 : 0.2966 kg/day K2CO3
Stream 303 : 59.32 kg/day Ethanol
Stream 403 : 4.7456 kg/day NaOH

Product Streams

Stream 801 : 1000 kg/day
- 986.37 kg/day PCE
- 13.63 kg/day Sodium Polycarboxylate

Reactor Volume Design and Costs

This presentation outlines the design considerations for reactors R101, R102, and R103, including volume calculations and capital costs. We aim to provide a clear understanding of the scale and investment required for each reactor.

Reactor Volume Specifications

Reactor R101

Designed for 59.32 kg of effluent per day, requiring 56.44 L of space. Factoring in a 70% fill capacity, a reactor space of 80.62 L is selected.

Reactor R102

Handles 1305.3366 kg of components daily, primarily Non-Neutralised PCE. With a PCE density of 1.11 kg/L, it needs approximately 1175.98 L, resulting in a 1679.97 L reactor.

Reactor R103

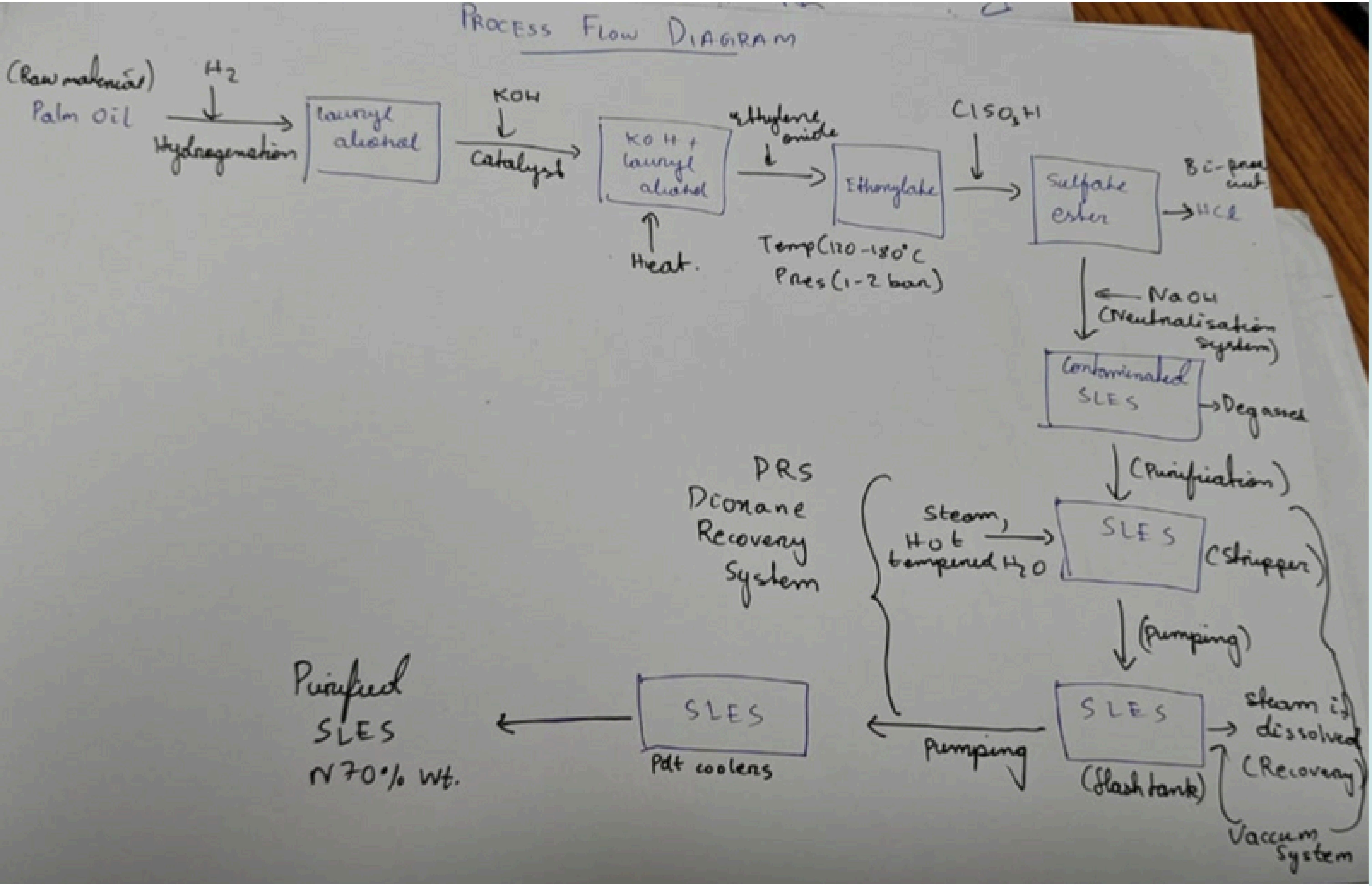
Processes 1000 kg of PCE, requiring 900.9 L of space. Considering the 70% fill capacity, a reactor space of 1285.714 L is chosen.

Capital Cost Analysis

Equipment	Capacity (L)	No. of units	Cost/unit ($ for year 2014)	Total Cost ($ for year 2014)
Reactor R101	80.62	1	6,100	6,100
Reactor R102	1679.97	1	30,500	30,500
Reactor R103	1285.714	1	4,800	4,800
			Total	41,400 USD

SLES

PFD



PROCESS FLOW DIAGRAM
(Raw material)
Palm Oil
H2
Hydrogenation
lauryl alcohol
KOH
Catalyst
KOH + lauryl alcohol
Heat.
ethylene oxide
Ethoxylate
Temp(120-180°C
Pres(1-2 bar)
ClSO3H
Sulfate ester
HCl
NaOH
(Neutralisation system)
Contaminated SLES
Degassed
(Purification)
PRS
Dioxane
Recovery
System
Steam,
Hot
tempered H2O
SLES
(Stripper)
(Pumping)
SLES
(flash tank)
Steam if dissolved
(Recovery)
Vaccum
System
Pumping
SLES
Pdt coolers
Purified
SLES
~70% Wt.

Reaction Process Conditions (For SLES)

Hydrogenation

Requires controlled temperature and pressure in the presence of a catalyst (typically Ni, Pd, or Pt) to add hydrogen atoms, reducing unsaturated bonds in the compound.

Ethoxylation

Involves the reaction of ethylene oxide with an alcohol or phenol under controlled temperature and pressure, typically with a catalyst, to introduce ethoxy groups.

Sulfation

Requires reaction with sulfur trioxide (SO_3) or chlorosulfonic acid under regulated conditions to introduce sulfate groups, forming surfactant precursors.

Neutralization

Requires pH control to ensure complete neutralization of acidic groups (e.g., sulfate or carboxylic acid groups), typically around pH 6–7, for optimal stability and performance.

Separation and Purification Techniques

Phase Separation (Decanter)

Decantation is used to separate unreacted oils or hydrophobic impurities from the aqueous SLES phase based on density differences.

Filtration

Remove solid impurities or catalyst residues from the ethoxylated alcohol or sulfated mixture.

Evaporation (Vacuum System)

Remove volatile components, mainly water or excess ethanol (if used), under reduced pressure.

Purification (Membrane/Stripping + PRS – Dioxane Recovery System)

Purify the SLES by removing organic traces, degraded surfactants, and other micro-contaminants.

Process

We scaled up the lab synthesis to a plant producing 1000 kg/day

Input Materials :

- Palm Oil
- Hydrogen (H_2)
- Ethylene Oxide (EO)
- Sulfur Trioxide (SO_3)
- Sodium Hydroxide (NaOH)
- Catalyst (KOH)
- Water
- Processing Additives (Cooling, Solvent, etc.)

Input Streams

- Palm Oil: 1200
- Hydrogen (H_2): 30
- KOH (Catalyst): 5
- Ethylene Oxide (EO): 490
- EO Catalyst: 2
- Sulfur Trioxide (SO_3): 360
- Solvent Medium: 50
- Sodium Hydroxide (NaOH): 150
- Water & Additives (for dilution): 300

Product Streams

Purified SLES (70% solution): 1000

- SLES Active (Dry Basis): 700.00 kg/day
- Water & Additives in SLES: 300.00 kg/day

Reactor Volume Specifications

Hydrogenation

Designed to process 980 kg/day of lauryl alcohol. This requires approximately 933.33 L of reactor space daily. Applying a 70% fill factor for operational safety, the reactor volume is calculated to be around 1333.33 L, leading to the selection of a 1500 L reactor.

Ethoxylation

Handles 1440 kg of lauryl ether alcohol per day through ethoxylation. With the required volume being 1371.43 L/day, and accountingaccounting for a 70% fill capacity, the selected reactor volume is 2530.61 L, rounded up to a 2000 L.a capacity required obtained to be 1959.18 , rounded up to 2000 L.

Sulfation

Processes 1740 kg/day of SLES acid form, requiring approximately 1657.14 L of working volume daily. Considering a 70% fill capacity, a reactor size of 2367.34 L is calculated. A 2500 L reactor is selected to accommodate this load.

Neutralization

Handles 1860 kg/day of crude SLES. This corresponds to a required working volume of approximately 1771.43 L per day. Accounting for a 70% fill capacity, the selected reactor volume is 2530.61 L, rounded up to a 2600 L reactor for operational safety and design flexibility.

CAPITAL COST ANALYSIS:

Step	Type of Reactor	Material of Reactor	No. of units	Design Capacity (L)	Internal Pressure (in psi)	Cost/unit (in US$ for year 2014)	Total Cost (in US$ for year 2014)
Hydrogenation	Autoclave	Glass-lined CS	1	1500	450 (high)	185,000	185,000
Ethoxylation	Jacketed, Agitated	Glass-lined CS	1	2000	100 (moderate)	46,200	46,200
Sulfation	Jacketed, Non-Agitated	Glass-lined CS	1	2500	75 (low)	9,300	9,300
Neutralization	Mixer/Settler	Glass-lined CS	1	2600	15 (atmospheric)	143,000	143,000

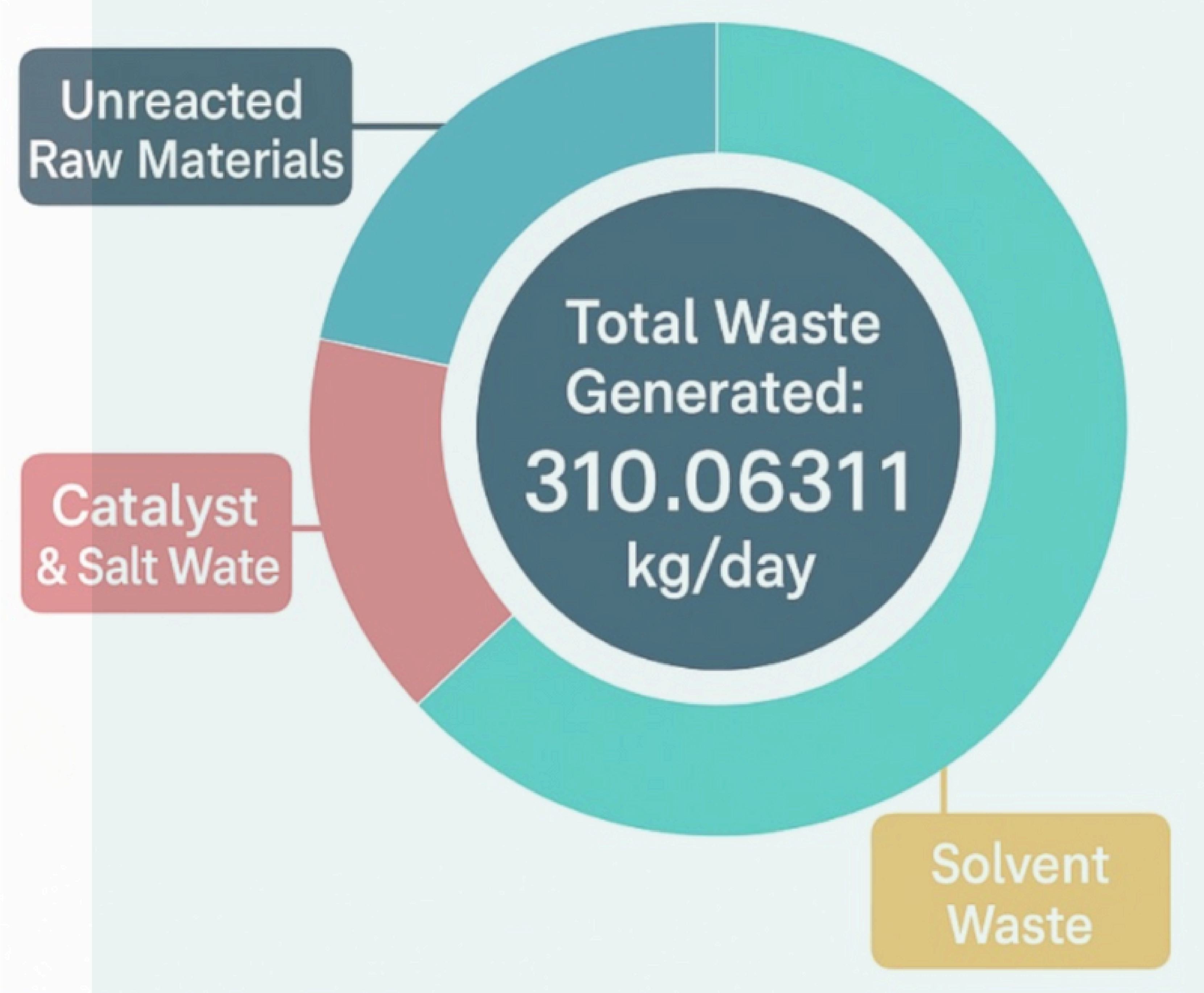
Total = 185,000 + 46,200 + 9,300 + 143,000 = 383,500 USD

ENVIRONMENT, HEALTH AND SAFETY

Introduction

Purpose:

- Chemical Product Formula: $CH_2=C(R)-COO-(CH_2CH_2O)_nR'$
- Product Name: Polycarboxylate Ether (PCE)
- Analyze waste generation during PCE production
- Classify waste by type and quantity
- Propose safer handling and reduction strategies



Waste Generation Overview

Types of Wastes:

- Unreacted Raw Materials
- Byproduct Water
- Catalyst & Salt Waste
- Solvent Waste

Total Waste Generated: 310.06311 kg/day

Types of Wastes Overview

Unreacted Raw Materials

Material	Waste Quantity (kg/day)	Stream	Source
Acrylic Acid (AA)	1.4237	802	R101
Methacrylic Acid (MA)	1.6610	802	R101
CMP	1.1271	802	R101

Solvent Waste

Material	Waste Quantity (kg/day)	Stream	Notes
Ethanol	59.32	702	Evaporated solvent

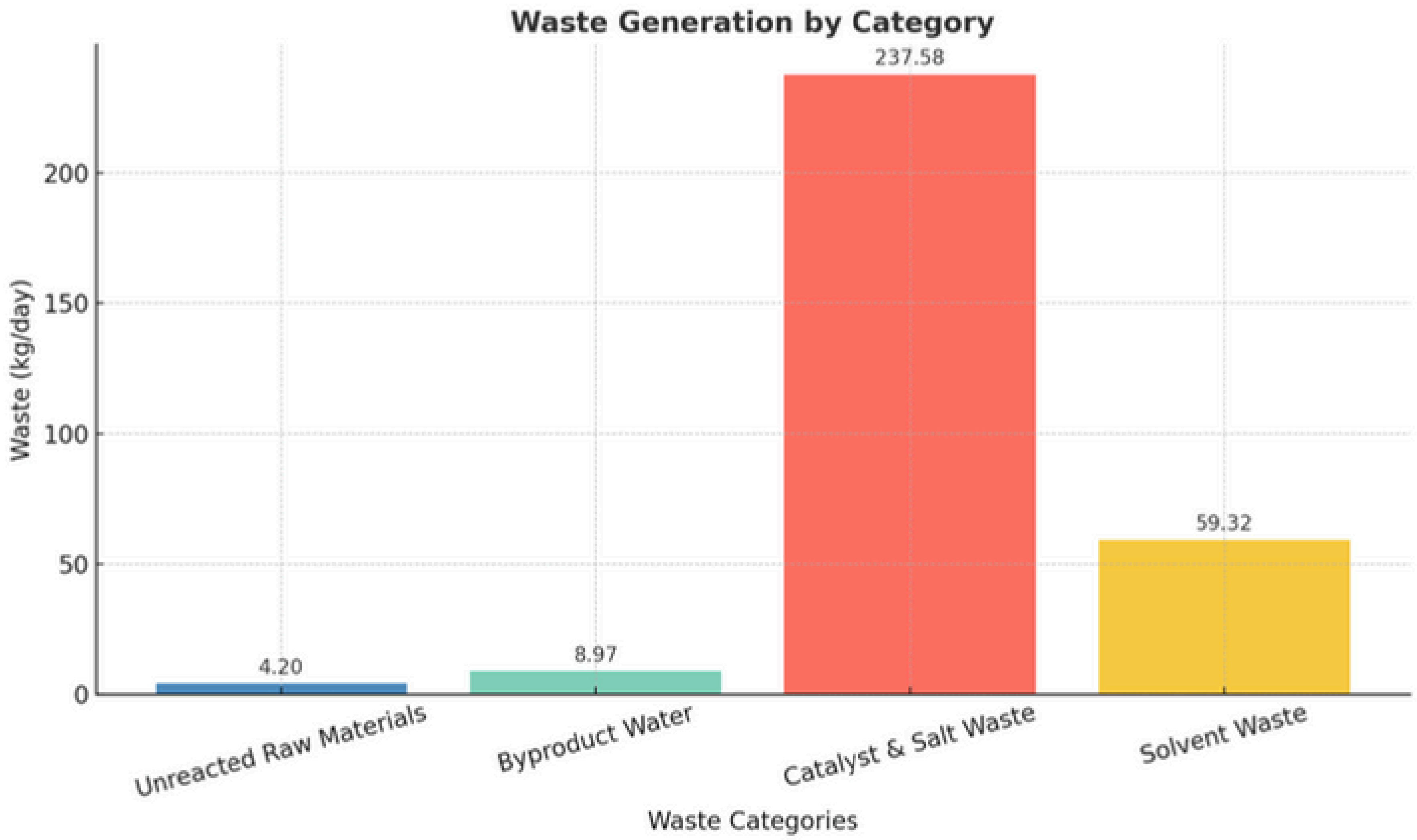
Byproduct Streams

Material	Waste Quantity (kg/day)	Stream	Notes
Water (Esterification)	6.8336	603	Byproduct water
Water (Neutralization)	2.1355	603	Reaction byproduct

Catalyst and Salt Waste

Material	Waste Quantity (kg/day)	Stream	Notes
K_2CO_3	0.2966	602	Filtered catalyst
MPEG	237.28	802	Unreacted

Graph – Waste Generation by Category



Insights:

- Catalyst & Salt Waste is the dominant contributor **(237.58 kg/day)**
- Focus required on MPEG recovery or reuse

Disposal Limits

S. No.	Parameter	Standards			
		Inland surface water	Public Sewers	Land for irrigation	Marine coastal areas
1	2	3			
		(a)	(b)	(c)	(d)
7.	Oil and grease mg/l Max.	10	20	10	20
8.	Total residual chlorin mg/l Max.	1.0	--	--	1.0
9.	Ammonical nitrogen (as N), mg/l Max.	50	50	--	50
10.	Total Kjeldahl Nitrogen (as NH_3) mg/l, Max.	100	--	--	100
11.	Free ammonia (as NH_3) mg/l, Max.	5.0	--	--	5.0
12.	Biochemical Oxygen demand [1][3 days at 27°C] mg/l max.	30	350	100	100
13.	Chemical Oxygen Demand, mg/l, max.	250	--	--	250
14.	Arsenic (as As), mg/l, max.	0.2	0.2	0.2	0.2
15.	Mercury (as Hg), mg/l, Max.	0.01	0.01	--	0.01
16.	Lead (as Pb) mg/l, Max.	0.1	1.0	--	2.0
17.	Cadmium (as Cd) mg/l, Max.	2.0	1.0	--	2.0
18.	Hexavalent Chromium (as Cr+6), mg/l max.	0.1	2.0	--	1.0

https://cpcb.nic.in/GeneralStandards.pdf

S. No.	Parameter	Standards			
		Inland surface water	Public Sewers	Land for irrigation	Marine coastal areas
12.	Biochemical Oxygen demand [1][3 days at 27°C] mg/l max.	30	350	100	100
13.	Chemical Oxygen Demand, mg/l, max.	250	--	--	250
5.	pH Value	5.5 to 9.0	5.5 to 9.0	5.5 to 9.0	5.5 to 9.0

Disposal Limits

As such, disposal limits for any of the waste/effluents mentioned in the whole process were not mentioned in any government or reliable sites officially.

General disposal limits were available in **The Environment Protection Rules, 1986** by **Central Pollution Control Board (under MoEFCC)**

which is one of the primary legislative frameworks for setting environmental standards, including:

- Effluent discharge norms
- Emission standards
- General environmental procedures
- Pollutant limits

[1][SCHEDULE – VI]
(See rule 3A)

GENERAL STANDARDS FOR DISCHARGE OF ENVIRONMENTAL POLLUTANTS PART-A : EFFLUENTS

S. No.	Parameter	Standards			
		Inland surface water	Public Sewers	Land for irrigation	Marine coastal areas
1	2	3			
		(a)	(b)	(c)	(d)
1.	Colour and odour	See 6 of Annexure-I	--	See 6 of Annexure -I	See 6 of Annexure-I
2.	Suspended solids mg/l, Max.	100	600	200	(a) For process waste water- 100 (b) For cooling water effluent 10 percent above total suspended matter of influent.
3.	Particulate size of suspended solids	Shall pass 850 micron IS Sieve	--	--	(a) Floatable solids, max. 3 mm. (b) Settleable solids, max. 850 microns.
[2]4.	***	*	--	***	--
5.	pH Value	5.5 to 9.0	5.5 to 9.0	5.5 to 9.0	5.5 to 9.0
6.	Temperature	shall not exceed 5°C above the receiving water temperature	--	--	shall not exceed 5°C above the receiving water temperature

Waste Treatment

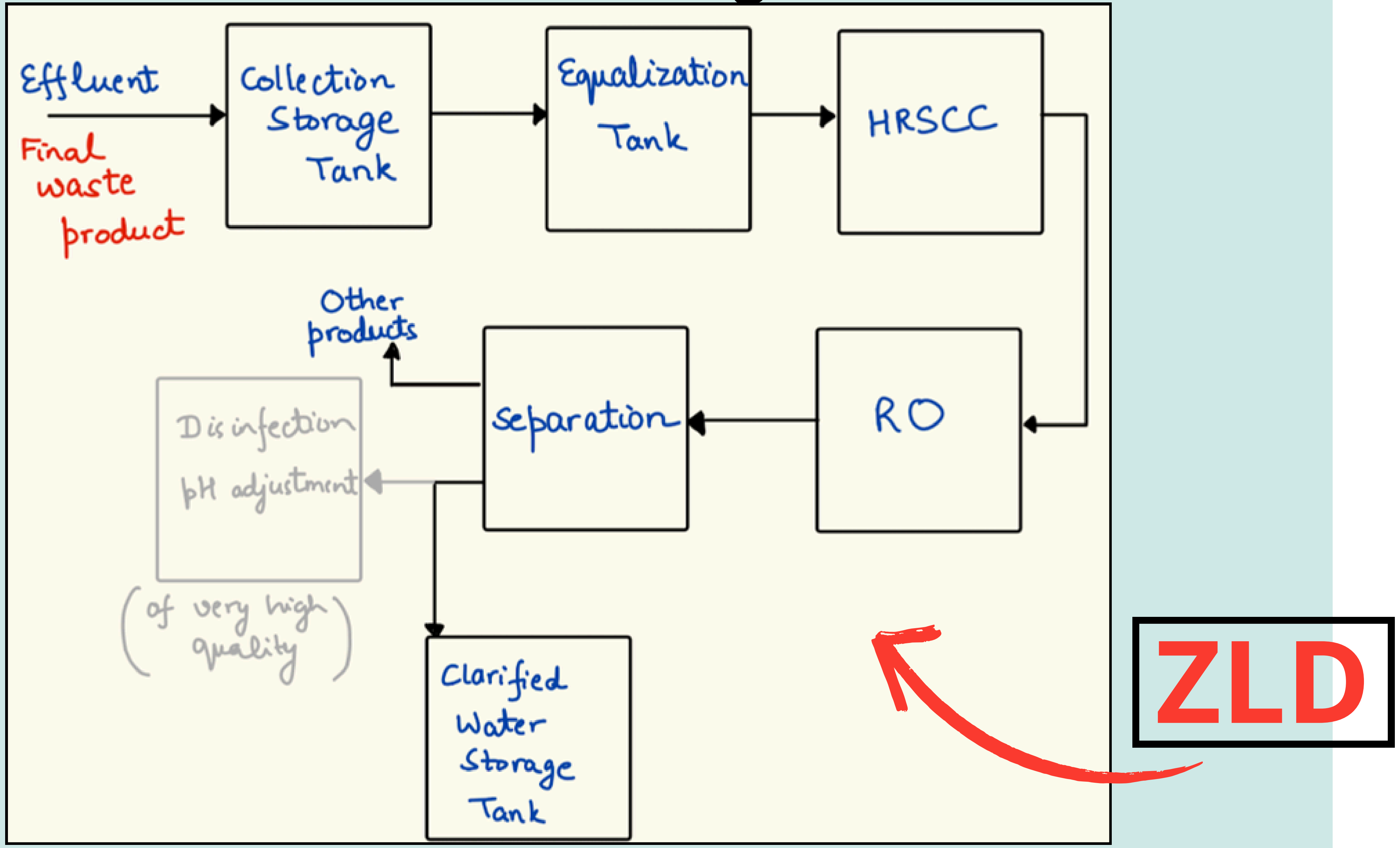
Liquid wastes: Waste Water, Ethanol, CMP, acrylic acid, methacrylic acid, MPEG (lower).

- Ethanol, CMP, acrylic acid, etc, can be used again as reactants.
- Thus, only separation is enough for them.
- Waste water needs to be treated, ensuring disposal limits and zero liquid discharge.

Idea:

We need to separate reactants (so that we can send them back to feed) and wastewater from the effluent.

Overall Block Diagram



Waste Treatment

Process:

Steps:

1. Collection Tank
2. Equalization Tank
3. HRSCC
4. RO
5. Distillation
6. Clarified Water

Not necessary (FOR CATALYST RECOVERY)

Distillation:

Distillation, here, is not that simple.

Since our waste liquid contains multiple reactant and product wastes, we need to separate all of them to reuse/store/treat them

The water recovered from distillation is ready to use in various processes.

Potential use cases:

- Heat exchangers.
- Irrigation.
- Personal, Domestic use (after pH treatment, disinfectant, etc)
- Industrial application
- and many more

Precaution:

Avoid mixing CMP and Ethanol:

- Both of them are miscible and have very close boiling points (difference of about 7 celsius)
- It will be an arduous task to separate them.

Solution:

Separate CMP before the introduction of ethanol stream.

Distillation

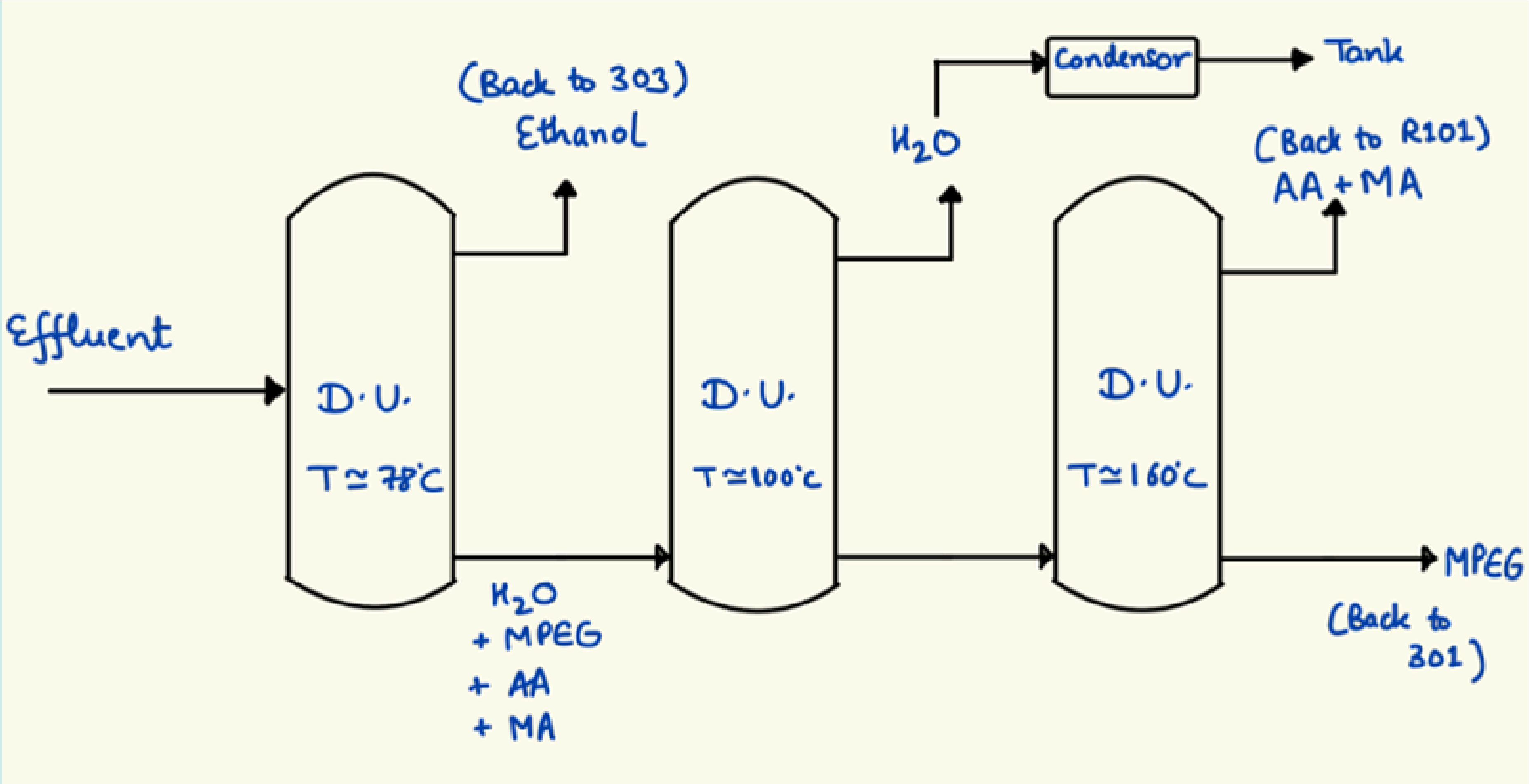
Boiling point:

Ethanol: 78°C.

Water: 100°C. For reuse (ZLD).

Acrylic & Methacrylic Acid: 141 & 161°C, respectively.

MPEG- Higher bp (more than 250 °C), remains liquid.



<u>Process</u>

Selective Vaporization

Control the temperature to separate components based on their bp.

Order of distillation:

- Ethanol Recovery
- Water Distillation: Directed to a Zero Liquid Discharge (ZLD) system.
- Acid Separation(Acrylic Acid (AA) & Methacrylic Acid (MA)
- MPEG: With a higher boiling point, MPEG remains as a liquid

CMP separation

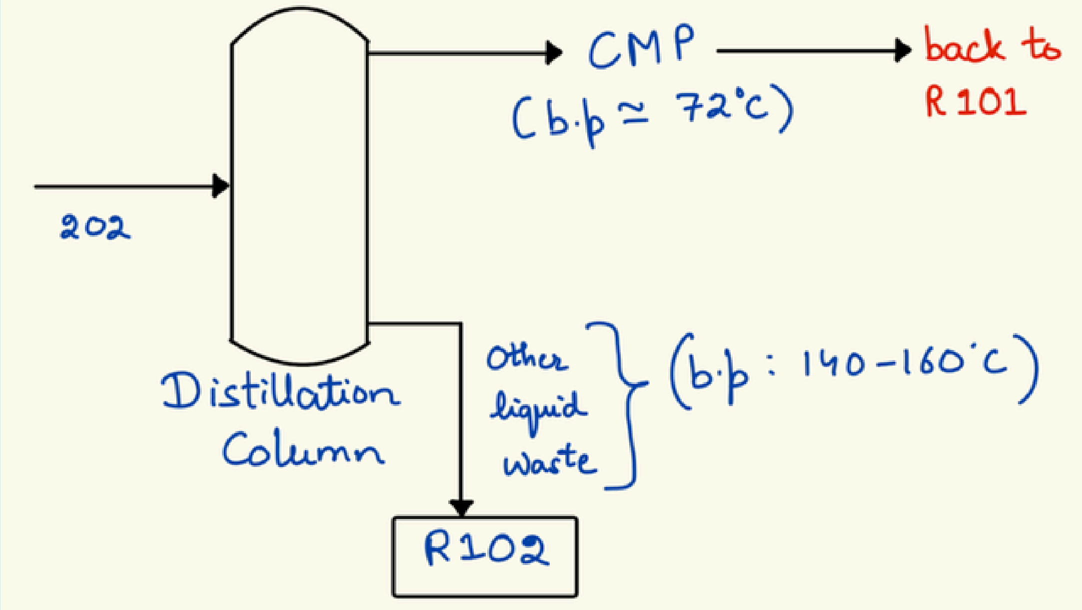
Objective: Recover pure CMP from stream 202, which also contains Acrylic Acid (AA) and Maleic Anhydride (MA).

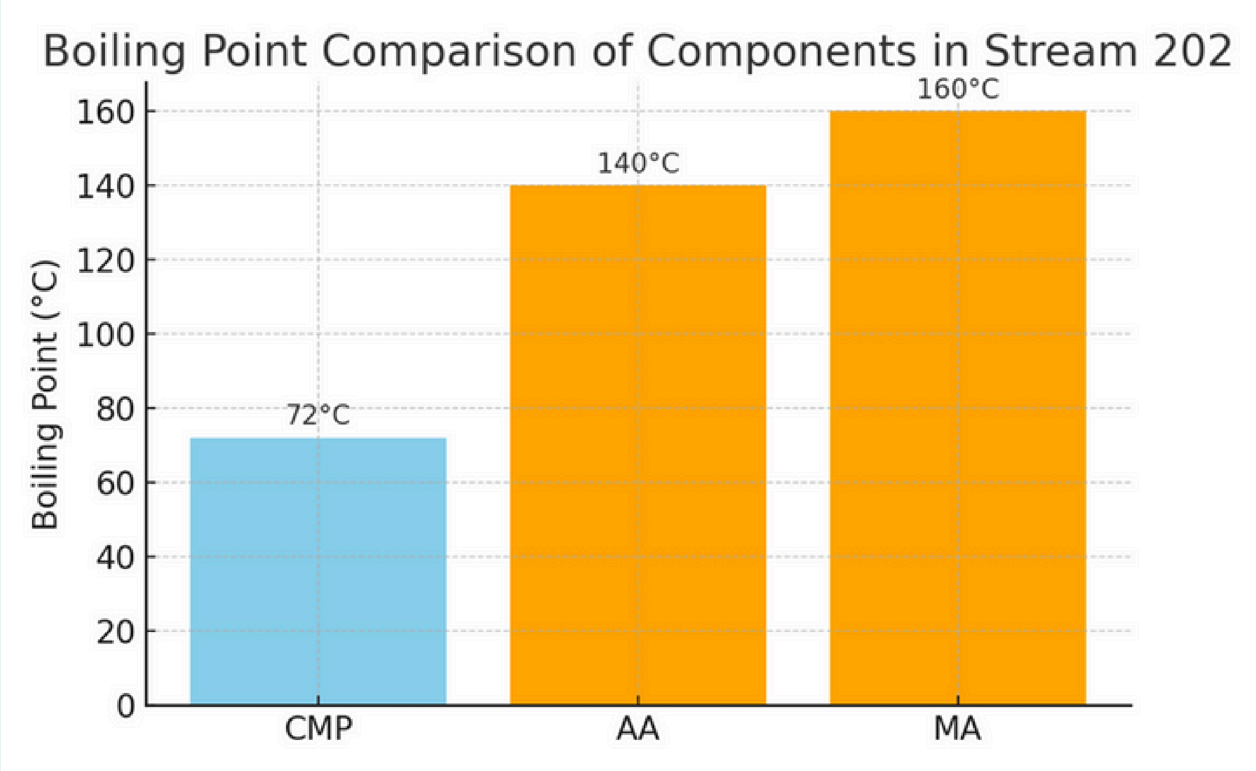
Separation Principle:

- Utilizes the difference in boiling points:
- CMP: ~72°C
- AA: ~140°C
- MA: ~160°C

Process Flow:

- Stream 202 is fed into a distillation column.
- CMP, having the lowest boiling point, is distilled off first and sent back to R101 for reuse.
- Heavier components (AA and MA) are directed to R102 as liquid waste.





TWA vs STEL

TWA is the average exposure to a hazardous substance over a normal 8-hour workday and 40-hour workweek.

Importance:

Helps limit chronic exposure to harmful substances.
Ensures workers stay within safe daily limits over long periods.

STEL is the maximum concentration of a hazardous substance a worker can be exposed to for a short time (usually 15 minutes) without harm.

Importance:

- Protects against short bursts of high exposure that can still be dangerous even if TWA is within limits.
- Especially important for irritants or fast-acting toxins.

TABLE

Chemical	TWA (8 hours)	STEL (15 minutes)
Ethanol	1000 ppm (OSHA PEL, NIOSH REL)	1000 ppm (ACGIH TLV-STEL)
Methoxy Polyethylene Glycol	No mention in any reliable source.	No mention in any reliable source.
Acrylic Acid	2 ppm (NIOSH REL, ACGIH TLV-TWA)OEL (Occupational Exposure Limit) EU: 10 ppm (29 mg/m³) over an 8-hour TWA.	DOSH: 20 ppm (59 mg/m³) averaged over a 15-minute period. [2]
Methacrylic Acid	20 ppm (NIOSH REL, OSHA PEL, ACGIH TLV-TWA)	No mention in any reliable source.
3-Chloro-2-methyl-1-propene	No mention in any reliable source.	0.3 mg/m3 [4, only mention across all websites]

Safety Concerns & Precautions

Safety Hazards

- **Ethanol**
  - Highly flammable
  - Inhalation: dizziness, drowsiness
  - Long-term: liver & nerve damage
- **Methoxy Polyethylene Glycol**
  - **Generally safe**
  - Irritates skin/eyes at high levels
  - May foam in water, releases formaldehyde when heated
- **Acrylic and Methacrylic Acid**
  - Flammable, corrosive
  - Inhalation toxic
  - Risk of polymerization
- **3-Chloro-2-methyl-1-propene**
  - Flammable & toxic (inhalation/ingestion/skin)
  - Group 3 carcinogen
  - Harmful to aquatic life

Precautions

- **Ethanol**
  - Keep away from heat
  - Store tightly sealed
- **Methoxy Polyethylene Glycol**
  - Use gloves for concentrated forms
  - Store at room temp, away from oxidizers
- **Acrylic Acid**
  - Store below 15 °C
  - Use PPE, ensure ventilation
- **Methacrylic Acid**
  - Store with inhibitor (e.g., hydroquinone)
  - Use PPE, avoid heat/oxidizers
- **3-Chloro-2-methyl-1-propene**
  - Handle in fume hood with PPE
  - Store cold, dry, away from oxidizers

THANK YOU