Invention: Chemical molecule and synthesis route

Applicant: QuantiVEX

Inventors: Aditya Nitin Patil

Chemical Formula: $RO(CH_2CH_2O)nH$

Chemical Name: Fatty Alcohol Ethoxylates

Chemical synthesis routes:

Ethoxylation of fatty alcohols:

The production of **Fatty Alcohol Ethoxylates (FAE)** involves the ethoxylation of fatty alcohols, where fatty alcohols (derived from natural oils or petrochemicals) are reacted with **ethylene oxide (EO)** in the presence of a **catalyst such as potassium hydroxide (KOH)** or specialized narrow-range catalysts. The process is typically carried out in a pressurized reactor at controlled temperatures (120-180°C) to ensure optimal reaction efficiency and product quality. The number of EO units added determines the **hydrophilic-lipophilic balance (HLB)** and the final product's properties. Post-reaction steps may include neutralization, purification, and stabilization to enhance product stability and performance. This method is widely used due to its efficiency, scalability, and ability to produce FAEs with tailored properties for various industrial applications.

RAW MATERIALS:

a. **Fatty Alcohols –** Can vary in chain length, typically between C8 to C18.
b. **Ethylene Oxide (EO) –** Reacts with fatty alcohols to form the ethoxylate chains.
c. **Catalyst –** Alkaline Catalysts – e.g., Potassium Hydroxide (KOH), Sodium Hydroxide (NaOH).
   Specialized Catalysts – e.g., Calcined Layered Double Hydroxides (LDHs) for narrow-range ethoxylates (NREs).
d. **Stabilizers/Inhibitors –** Added to control unwanted side reactions (e.g., polymerization of ethylene oxide).
e. **Neutralizing Agents (Post-Reaction) –** Common agents like phosphoric acid or acetic acid are used to neutralize residual catalysts.

UTILITIES REQUIRED:

1. stainless steel, high-pressure, and high-temperature batch or semi-batch reactor with agitation.
2. Steam Generation System
3. Ethylene Oxide Storage and Handling System (EO Storage Tanks, EO Flow Control Units, EO Scrubbers and Vent Systems)
4. Feedstock Preheating and Mixing Units
5. Gas Handling and Ventilation (Nitrogen, hydrogen and carbon monoxide supply)
6. Cooling System, Chillers
7. Stripping and Purification Columns
8. Neutralization and Post-Treatment Units
9. Storage Tanks
10. Advanced Distributed Control Systems (DCS) or Programmable Logic Controllers (PLCs)
11. Safety and Environmental Unit

<u>CHEMICAL PROCESSES:</u>

Step 1: Production of Fatty Alcohols

Fatty alcohols serve as the primary substrates for FAE synthesis. They can be derived through various methods:

1. **Hydrogenation of Fatty acids or Fatty acid esters**
    - <u>Fatty acid formation:</u>

      Hydrolysis of Triglycerides:

      $(C_{17}H_{35}COO)_3C_3H_5 + 3H_2O \rightarrow 3C_{17}H_{35}COOH + C_3H_8O_3$

    - <u>Hydrogenation of Fatty acids/ Fatty acid esters:</u>

      Hydrogenation of Fatty Acids:

      $R{-}COOH + 2H_2 \rightarrow R{-}CH_2OH + H_2O$

      Catalysts: Nickel (Ni), Copper-Chromium (Cu/Cr), or Copper-Zinc (Cu/Zn)

      Temperature Range: 150-250°C

      Pressure Range: 100-300 psi

2. **Oxo Process (Hydroformylation + Hydrogenation):**

This process is commonly used for producing **branched** and **linear fatty alcohols** from **olefins**.

- Hydroformylation (Oxo Reaction):

  $R{-}CH{=}CH_2 + CO + H_2 \rightarrow R{-}CH_2{-}CH_2{-}CHO$

  catalysts: Cobalt, Rhodium

- Hydrogenation of Aldehydes:

  $R{-}CH_2{-}CH_2{-}CHO + H_2 \rightarrow R{-}CH_2{-}CH_2{-}CH_2OH$

  catalysts: Nickel, Palladium, Platinum

4. **Ziegler Process (Ethylene Chain Growth Process):**

   This method is particularly effective for producing **high-purity linear fatty alcohols**.

   - Formation of Alkyl Aluminum Intermediate:

     $Al(C_2H_5)_3 + nC_2H_4 \rightarrow Al(C_2H_5)(C_nH_{2n+1})_2$

   - Oxidation:

     $Al(C_2H_5)(C_nH_{2n+1})_2 + O_2 \rightarrow Al(OC_nH_{2n+1})_3$

   - Hydrolysis:

     $Al(OC_nH_{2n+1})_3 + 3H_2O \rightarrow 3R{-}OH + Al(OH)_3$

Process Efficiency:

- **Yield**: ~90-98%
- **Hydrogenation Process:** Achieves higher purity (~99%) for linear fatty alcohols.
- **Oxo Process:** Slightly lower purity (~95-97%) due to branched isomers.
- **Ziegler Process:** Yields extremely pure linear fatty alcohols (~98-99%) but is complex and costly.

Step 2: Catalyst Activation and Alkoxide Formation

The first stage involves the reaction between the fatty alcohol and the alkali metal catalyst, resulting in the formation of an alkoxide ion — a powerful nucleophile essential for ethoxylation.

1. **Alkoxide Formation:**

   $R{-}OH + Na \rightarrow R{-}O{-}Na^+ + 1/2H_2$

The alkali metal reacts with the alcohol’s hydroxyl group (-OH), abstracting the proton and releasing hydrogen gas.

The resulting **alkoxide ion** (R-O$^-$) is a strong nucleophile, enabling controlled ethylene oxide addition.

Process Efficiency:

- Yield: ~98-99%
- Purity: ~95-98%
- Controlled catalyst-to-alcohol ratio (1:1 to 1.2:1) minimizes side reactions.
- Delayed addition of ethylene oxide (EO) until alkoxide formation is <75% complete improves purity.

Step 3: Ethoxylation Reactions:

1. **Nucleophilic Attack on Ethylene Oxide (EO):**

   $R{-}O^- + C_2H_4O \rightarrow R{-}O{-}CH_2CH_2O^-$

   The negatively charged oxygen in the alkoxide ion attacks the partially positive carbon in the EO ring.

   This breaks the strained 3-membered ring and forms a new C-O bond, generating a **new alkoxide intermediate**.

2. **Chain Propagation (Ethoxylate Chain Growth):**

   $R{-}O{-}(CH_2CH_2O)_n^- + C_2H_4O \rightarrow R{-}O{-}(CH_2CH_2O)_{n+1}^-$

   Each successive addition of EO extends the ethoxylate chain by **one ethylene oxide unit**.

   The chain length depends on reaction conditions, catalyst concentration, and EO availability.

3. **Termination (Protonation):**

   $R{-}O{-}(CH_2CH_2O)_n^- + H_2O \rightarrow R{-}O{-}(CH_2CH_2O)_nH + NaOH$

This final protonation step neutralizes the remaining alkoxide and stabilizes the ethoxylated alcohol.

- Controlled EO Addition: Introducing EO when alkoxide formation is <75% complete minimizes PEG by-products.
- Narrow Temperature Range: Maintaining 100-150°C avoids EO degradation.
- Correct Catalyst Ratio: Ensuring a **1:1 molar ratio** between fatty alcohol and catalyst minimizes side reactions.
- Reaction Time: Ethoxylation typically occurs over **2-4 hours** for optimal control.

Process Efficiency:

- Yield: ~90-95% (with controlled conditions)
- Purity: ~92-98%
- Proper EO flow rate and controlled temperature (100-150°C) reduce polyethylene glycol (PEG) formation.
- Steam distillation improves product purity by removing unreacted fatty alcohols.

Step 4: Separation and Purification Processes:

The production of fatty alcohol ethoxylates (FAEs) involves several key separation and purification steps to ensure product quality and performance. Below is an overview of these processes:

1. Removal of Unreacted Fatty Alcohols:

Unreacted fatty alcohols can be separated from the ethoxylation mixture through distillation. This process involves heating the mixture to a temperature at least 20°C below the boiling point of the desired product, allowing the more volatile unreacted alcohols to be distilled off.

2. Elimination of Catalyst Residues:

Post-ethoxylation, residual catalysts such as potassium hydroxide (KOH) need to be neutralized and removed. This is typically achieved by adding a neutralizing agent, followed by filtration to eliminate any precipitated salts.

3. Separation of By-products:

By-products like polyethylene glycol (PEG) can form during ethoxylation. These are often separated using liquid-liquid extraction methods. For instance, ethyl acetate has been employed to extract FAEs from aqueous matrices, effectively separating them from PEGs.

4. Purification of Specific FAE Homologues:

To isolate specific homologues of FAEs, advanced chromatographic techniques are utilized. Liquid chromatography coupled with mass spectrometry (LC-MS) has been employed to separate and identify homogeneous FAE homologues, enabling precise analysis and purification.

5. Removal of Ionic Impurities:

Strong anion exchange (SAX) chromatography can be used to separate ionic impurities from FAEs. In this method, alkylether sulfates (AES), which are anionic, are retained on the SAX column, allowing the nonionic FAEs to be eluted and collected separately.

Process Efficiency:

- Yield: ~85-95% (depends on purification intensity)
- Purity: ~96-99%
- Steam Stripping efficiently removes unreacted fatty alcohols (purity ~98-99%).
- Liquid-liquid extraction effectively removes excess polyethylene glycol.
- Chromatographic separation is used in specialty-grade ethoxylates for achieving >99% purity.

References:

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List the contributions of each author:

1. **Aditya Nitin Patil** worked on selection of the chemical and selection of the manufacturing processes and studying the process, doing its manufacturing analysis and other factors.

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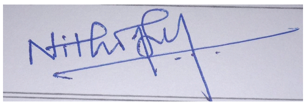
Nithin T M (CEO)	230709	
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