Nature of Invention: Chemical molecule and synthesis route

Applicant: ***GreenovateX***

Inventors: ***Shubham Agarwal***

Chemical Formula: ***C18H35N2NaO4***

Chemical Name: ***Sodium Lauroamphoacetate***

Chemical synthesis routes:

1) For lab scale preparation through Amidification method

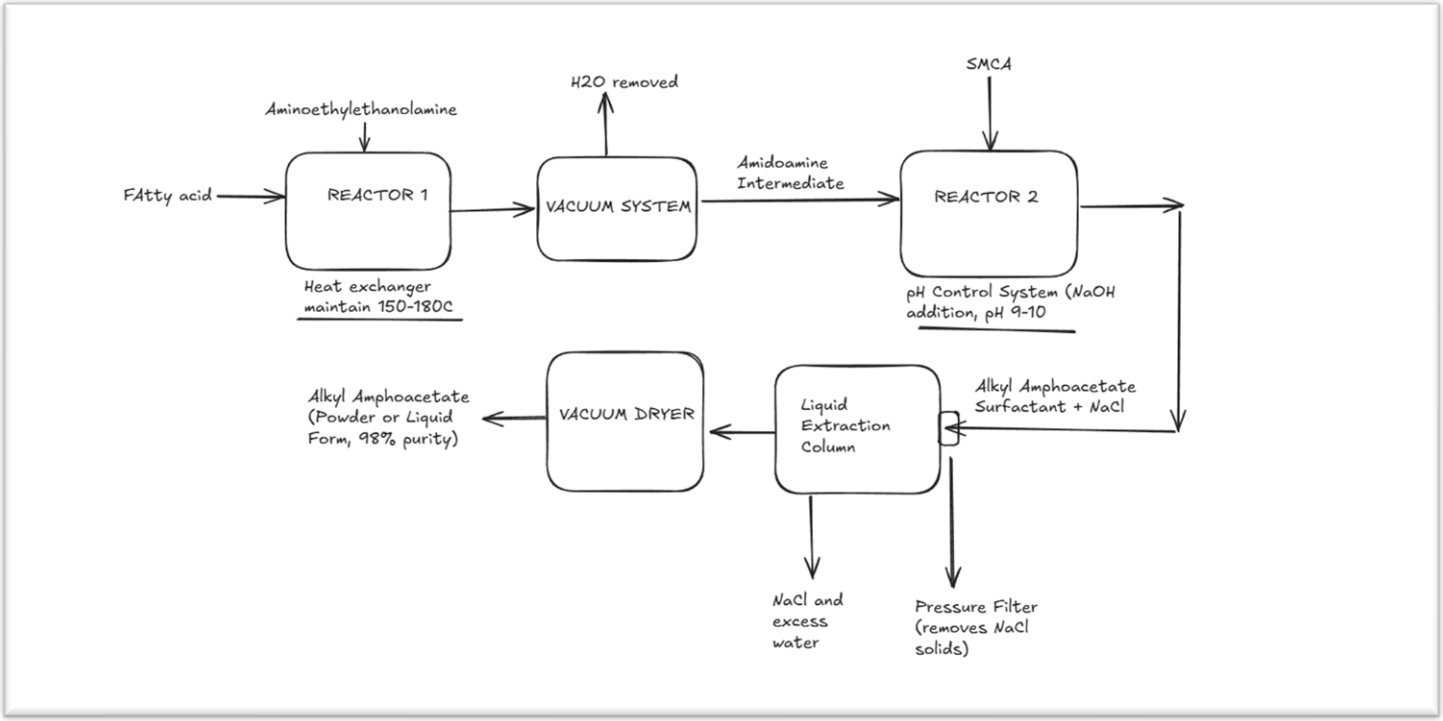
Chemicals required

- Fatty Acid
- Aminoethylethanolamine (AEEA)
- Sodium Monochloroacetate (SMCA)
- Sodium Hydroxide (NaOH)
- Water (H2O)
- Ethanol(C2H5OH)

Vessels required

- Reaction: Stirred Tank Reactor, Heat Exchanger, Vacuum System, pH Controller.
- Separation & Purification: Nutsche Filter, Extraction Column, Evaporator.
- Drying & Storage: Spray Dryer, Holding Tanks.

Process analysis



STEP 1 Amidation Reaction (Formation of Amidoamine Intermediate)

Objective: Convert fatty acid into amidoamine.

Reaction :

$$RCOOH + H_2NCH_2CH_2NHCH_2CH_2OH \rightarrow RCONHCH_2CH_2NHCH_2CH_2OH + H_2O$$

Reaction Conditions:

- Temperature: 150-180°C
- Pressure: Reduced pressure (10-50 mbar)
- Reaction Time: 2-4 hours
- Catalyst: Excess AEEA (~5-10% excess)
- Continuous Stirring for uniform reaction.

Process Flow:

- Heated fatty acids and AEEA are mixed in a reactor with agitation.
- The system is maintained under vacuum to remove water formed during the reaction.
- The resulting amidoamine is cooled and transferred to the next reactor

STEP 2 Carboxymethylation Reaction (Formation of Alkyl Amphoacetate)

Objective: Introduce carboxymethyl (-CH_2COONa) group to amidoamine.

Reaction: (Using SMCA)

$$RCONHCH_2CH_2NHCH_2CH_2OH + ClCH_2COONa \rightarrow RCONHCH_2CH_2N(CH_2COONa)CH_2CH_2OH + NaCl$$

Reaction Conditions:

- Temperature: 80-100°C
- pH: Adjusted to 9-10 using NaOH solution.
- Reaction Time: 3-6 hours.
- Controlled Addition of SMCA / Cyanide + Formaldehyde to prevent side reactions.

Process Flow:

- The amidoamine intermediate is transferred to the carboxymethylation reactor.
- The reaction is initiated by adding SMCA gradually while maintaining pH.
- The solution is stirred until completion, then cooled before purification.

Step 4: Filtration & Purification

***Objective*:** Remove impurities like NaCl, excess reactants, and solvents.

Steps:

1. Filtration: Solid NaCl is removed via vacuum filtration.
2. Solvent Extraction (if used**):** Ethanol or water is used to extract the surfactant phase.
3. Distillation: Excess solvent or water is evaporated.

Process Flow:

- The reaction mixture is filtered to remove salts.
- The surfactant solution undergoes solvent extraction and is purified via distillation.

Step 5: Drying & Final Product Storage

Objective: Remove remaining moisture and store the final product.

Steps:

- Drying: The product is dried to achieve the desired consistency.
- Cooling & Storage: Final product is collected in tanks or packed into containers.

Process Flow:

- The purified product is dried under controlled conditions.
- The dried product is packed or stored as a liquid in holding tanks.

2)Alternate lab scale preparation using Sodium Cyanide

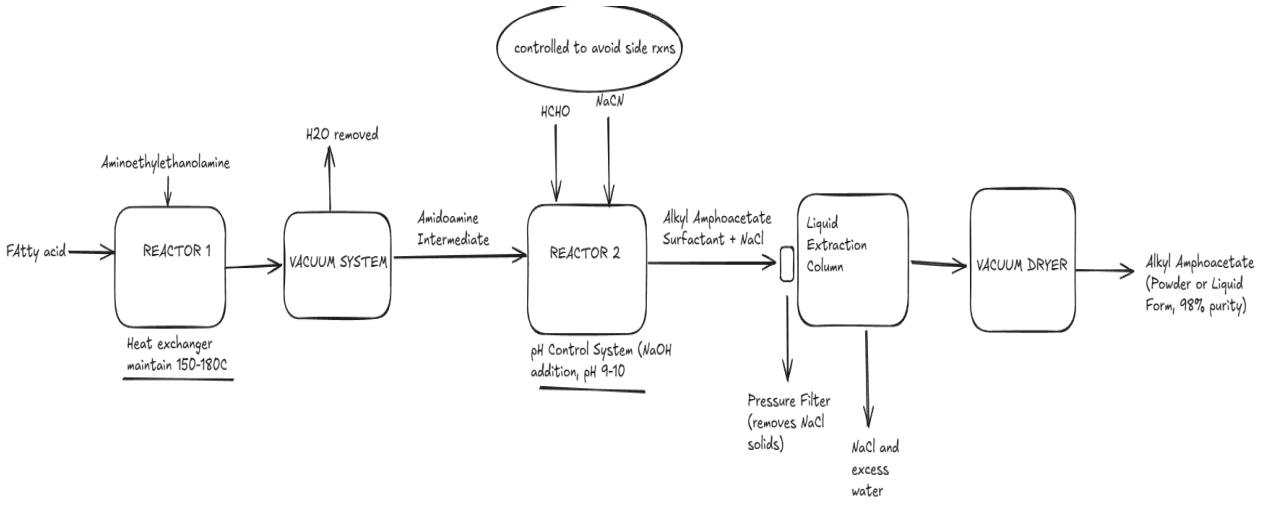
Chemicals required

- Fatty Acid (Lauric Acid, Coconut Fatty Acid, or Oleic Acid)
- Aminoethylethanolamine (AEEA)
- Sodium Cyanide (NaCN, solid or solution)
- Formaldehyde (HCHO, 37% solution)
- Sodium Hydroxide (NaOH, 30% solution)
- Hydrochloric Acid (HCl, diluted)
- Water (Deionized or Distilled)
- Ethanol or Isopropanol
- Sodium Chloride (NaCl)
- Hydrogen Peroxide (H_2O_2) or Sodium Hypochlorite (NaOCl)

Vessel required

- Storage Tanks
- Airtight Cyanide Storage Tank
- Jacketed Stirred Tank Reactor
- Vacuum System
- Heat Exchanger
- Nutsche Filter / Pressure Filter
- Liquid- Thin Film Evaporator
- Liquid Extraction Column

Process analysis



STEP 1 Amidation Reaction (Formation of Amidoamine Intermediate)

Objective: Synthesize the amidoamine intermediate from fatty acids and aminoethylethanolamine (AEEA).

Reaction: $RCOOH + H_2NCH_2CH_2NHCH_2CH_2OH \rightarrow RCONHCH_2CH_2NHCH_2CH_2OH + H_2O$

Process Conditions:

- Temperature: 150-180°C
- Pressure: Reduced pressure (10-50 mbar)
- Reaction Time: 2-4 hours
- Catalyst: Excess AEEA (~5-10% excess)
- Continuous stirring for uniform reaction

Process Flow:

- Heated fatty acids and AEEA are mixed in the reactor with agitation.
- The system is maintained under vacuum to remove water formed during the reaction.
- The resulting amidoamine is cooled and transferred to the next reactor.
-

STEP 2 Carboxymethylation Reaction (Formation of Alkyl Amphoacetate)

Objective: Introduce the carboxymethyl ($-CH_2COONa$) group to the amidoamine.

Reaction: $RCONHCH_2CH_2NHCH_2CH_2OH + HCHO + NaCN \rightarrow RCONHCH_2CH_2N(CH_2COONa)CH_2CH_2OH$

Process Conditions:

- Temperature: 80-100°C
- pH: Adjusted to 9-10 using NaOH solution
- Reaction Time: 3-6 hours
- Controlled addition of formaldehyde and sodium cyanide to prevent side reactions

Process Flow:

- The amidoamine intermediate is transferred to the carboxymethylation reactor.
- Formaldehyde and sodium cyanide are added gradually while maintaining pH.
- The solution is stirred until completion, then cooled before purification.

STEP 3 Filtration and Purification

Objective: Remove impurities like NaCl, excess reactants, and solvents.

Steps:

- Filtration: Solid NaCl is removed via vacuum filtration.
- Solvent Extraction (if used): Ethanol or water is used to extract the surfactant phase.
- Distillation: Excess solvent or water is evaporated.

Process Flow:

- The reaction mixture is filtered to remove salts.
- The surfactant solution undergoes solvent extraction and is purified via distillation.

STEP 4 Drying and Storage

Objective: Remove remaining moisture and store the final product.

Steps:

- Drying: The product is dried to achieve the desired consistency.
- Cooling & Storage: Final product is collected in tanks or packed into containers.

Process Flow:

- The purified product is dried under controlled conditions.
- The dried product is packed or stored as a liquid in holding tanks.

Reasons Why the Formaldehyde + Sodium Cyanide Carboxymethylation Route is Not Preferred

Although the Formaldehyde + Sodium Cyanide (NaCN) Carboxymethylation Route for alkyl amphoacetate production offers higher yield and lower raw material costs, it is less commonly used in industrial settings due to the following reasons:

- Sodium Cyanide (NaCN) is highly toxic, requiring airtight storage, full PPE, and strict handling protocols.
- Hydrogen Cyanide (HCN) risk due to cyanide reacting with acids or moisture, requiring scrubber systems to prevent gas leaks.
- Cyanide waste disposal is complex and requires neutralization with hydrogen peroxide (H_2O_2) or sodium hypochlorite (NaOCl) before safe discharge.
- Effluent treatment costs are high due to the need for cyanide oxidation units in ETP (Effluent Treatment Plants).
- Sodium cyanide and formaldehyde are restricted chemicals, requiring special handling permits and exposure monitoring.

- Strict compliance with CPCB (India), EPA (US), and REACH (EU) regulations increases operational complexity.
- High pH sensitivity (pH 11-12) requires continuous monitoring to avoid cyanide gas emissions.
- Side reactions (cyanohydrin formation) can lead to impurities, reducing final product purity and increasing purification steps.
- Although NaCN + Formaldehyde are cheaper than SMCA, the additional costs of safety systems, waste treatment, and regulatory compliance make the overall process more expensive.
- Investment in gas scrubbers, emergency response systems, and effluent treatment increases CAPEX & OPEX.

References:

https://patents.google.com/patent/US6232496B1/en

https://innospec.com/personal-care/surfactants/alkyl-amphoacetates/

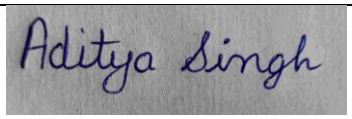
https://data.epo.org/publication-server/rest/v1.0/publication-dates/19990310/patents/EP0713860NWB1/document.html

https://www.freepatentsonline.com/6232496.html

https://patents.google.com/patent/WO2016199944A1/en

List the contributions of author: Shubham Agarwal

- Designed and implemented a chemical synthesis route for the production of Alkyl Amphoacetates, including raw material selection, process design, and optimization of key stages such as amidation, carboxymethylation, purification, and drying.
- Made the flowchart of both the process and added the crucial steps like vacuum system and pH control systems.
- Investigated about the alternate process using Cyanide and its whole flow diagram.
- Figured out which process is better and its reasoning which can be more friendly for company and production
- company and production

NAME	ROLL NO.	SIGNATURE
ADITYA SINGH	230079	
SHUBHAM AGARWAL	230996