FLUROXYPYR EHS

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CHEMICAL FORMULA	$C_7H_5Cl_2FN_2O_3$
CHEMICAL NAME	Fluroxypyr

Environmental, Health and Safety (EHS) Summary for Fluroxypyr Production

Fluroxypyr production involves several chemical processes with associated waste generation, regulatory considerations, treatment requirements, and safety concerns. This report addresses these aspects based on the production methods and mass balance data provided.

a. List the wastes generated and their quantity of generation
The production of Fluroxypyr generates multiple waste streams through its synthesis pathways. Based on the mass balance data and synthesis methodology, the following wastes are generated:

Waste Stream	Quantity (kg)	Source
Unreacted 4-Amino-3,5-dichloro-2,6-difluoropyridine	75.9	Remaining after 92% reaction completion
Unreacted Ethyl Glycolate	43.7	Remains after reaction
Water (produced during reaction)	79.1	Reaction byproduct
Excess K_2CO_3	184.75	Catalyst/base used in excess
TBAI (catalyst waste)	88.2 (13.2 lost)	Phase transfer catalyst
Hydrated $Na_2SO_4{\cdot}10H_2O$	118.65	Drying agent waste
Ethanol (from hydrolysis)	198.3	Byproduct of ester hydrolysis
NaCl (from acidification)	73.6	Byproduct of final acidification

Data for Fluroxypyr Production: -

- Desired Product: Fluroxypyr Ethyl Ester
- Mass: 1382.0 kg

Waste Streams:

- Unreacted 4-Amino-3,5-dichloro-2,6-difluoropyridine: 75.9 Kg
- Unreacted Ethyl Glycolate: 43.7 kg
- Water (produced during reaction): 79.1 kg
- Excess K2CO3K2CO3: 184.75 kg
- TBAI (catalyst waste): 88.2 kg
- Hydrated Na2SO4 · 10H2ONa2SO4 · 10H2O: 118.65 kg
- Ethanol (from hydrolysis): 198.3 kg
- NaCl (from acidification): 73.6 kg

Total Waste Mass:
Sum of all waste streams =
75.9+43.7+79.1+184.75+88.2+118.65+198.3+73.6=862.2 kg

Total Reactants Mass:
Desired product mass + Total waste mass = 1382.0+862.2=2244.2 Kg

Calculations:-

1.Atom Economy:

Using the formula:
Atom Economy=(Mass of Desired Product/Total Mass of Reactants)×100

Substituting values:

Atom Economy=(1382.0/2244.2)×100=**61.58%**

2.E-Factor:

Using the formula:
E-Factor=Total Mass of Waste/Mass of Desired Product

Substituting values:

E-Factor=862.2/1382.0=0.624

3.EQ Factor:

Assuming Q=2.5 for simplicity purposes (considering moderate impact)
Using the formula:

EQ-Factor= E-Factor × Q
Substituting values:

EQ-Factor=1.56

The waste materials generated during Fluroxypyr production are subject to various regulatory requirements:

Organic Solvents

- Toluene : Classified as F005 and U220 under RCRA regulations. Unused toluene (U220) must not be disposed of down drains or in regular trash. Used toluene (F005) must be treated as flammable hazardous waste. Triple-rinsing of containers is required before disposal

- Ethanol: Classified as D001 (flammable hazardous waste). Must be disposed of as hazardous waste for large amounts. Small amounts can be evaporated in a fume hood, followed by rinsing and proper disposal of containers

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Chemical Wastes

- Sodium Hydroxide: Corrosive waste (D002), must be separated from organic solvents whenever possible
- Potassium Carbonate: While not specifically regulated, as a basic compound it should be neutralized before disposal.
- Aqueous solutions: Those containing RCRA regulated toxic chemicals must be disposed of through hazardous waste management programs and not down drains

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Waste Segregation Requirements

- Corrosive wastes should be separated from organic solvents
- Nonhalogenated organic solvents should be separated from halogenated organic solvents
- Containers must be properly labeled and sealed to prevent spillage

c. Describe the treatment procedure for wastes with block diagram. Your chemical plant must be a zero liquid discharge plant.

Treatment Procedure for Zero Liquid Discharge Plant

<u>1. Two-Layer Separation System</u>

The reaction mixture forms two distinct layers after the esterification reaction:

- Organic Phase: Contains toluene, product (Fluroxypyr Ethyl Ester), and unreacted 4-Amino
- Aqueous Phase: Contains water, K_2CO_3, TBAI, and unreacted Ethyl Glycolate

<u>2. Aqueous Phase Treatment</u>

- Recovery of catalysts: K_2CO_3 (80% recovery) and TBAI (85% recovery) through precipitation
- Neutralization of remaining basic compounds

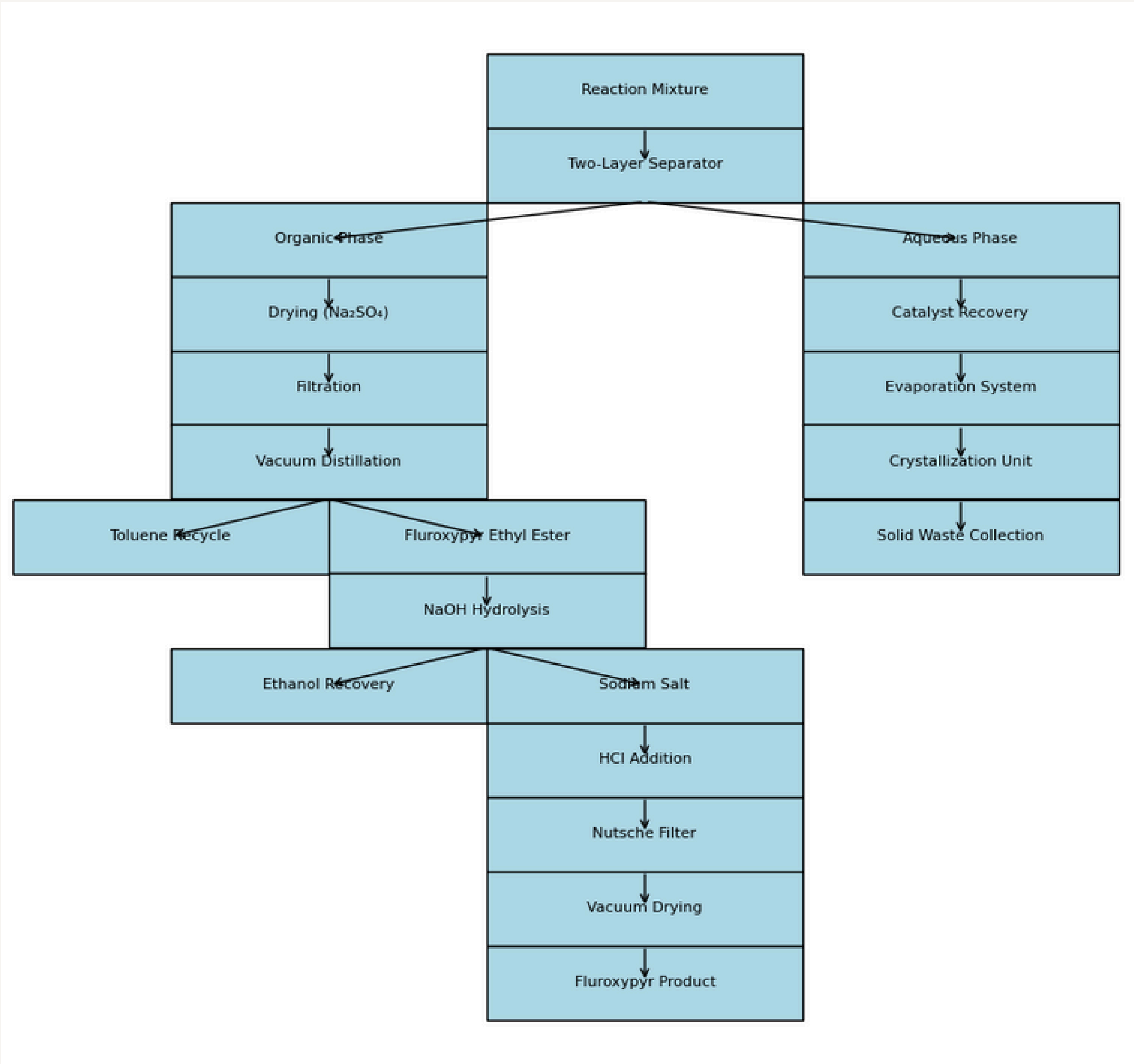
- Water treatment via multi-effect evaporation
- Crystallization of dissolved solids for recovery/disposal

3. Organic Phase Treatment
- Water removal using Na_2SO_4 (39.55 kg required for 79.1 kg water)
- Filtration to remove hydrated $Na_2SO_4 \cdot 10H_2O$ (118.65 kg)
- Vacuum distillation to recover toluene (8,227.0 kg, 100% recovery)
- Collection of Fluroxypyr Ethyl Ester (1,382.0 kg)

4. Hydrolysis Process Treatment
- Reaction of Fluroxypyr Ethyl Ester with NaOH (98% yield)
- Ethanol recovery through distillation (198.3 kg)
- Acidification with HCl to pH 1-2 to precipitate Fluroxypyr
- Collection of NaCl byproduct (73.6 kg)

5. Final Product Isolation
- Filtration using Nutsche filter
- Vacuum drying at 50°C for 6 hours
- Final product collection (high purity >95%)

Block Diagram for Zero Liquid Discharge System



Explanation of Safety Concerns and Exposure Limits for Chemicals

The chemicals involved in the production of Fluroxypyr present various safety concerns due to their hazardous nature. Below is a detailed explanation of their exposure limits and associated risks:

1. **Toluene**
   - Time Weighted Average (TWA):
   - OSHA: 200 ppm (8-hour TWA)
   - NIOSH: 100 ppm (8-hour TWA)
   - ACGIH: 20 ppm (8-hour TWA, stricter to prevent reproductive effects)
   - Short-Term Exposure Limit (STEL):
   - OSHA: 300 ppm (15-minute STEL)
   - NIOSH: 150 ppm (15-minute STEL)

Health Hazards:
- Toluene is a flammable liquid that can irritate the nose, throat, and respiratory system.
- Prolonged exposure may affect the nervous system, causing dizziness, headaches, and confusion.
- Chronic exposure can lead to liver, kidney, and brain damage.
- Safety Measures:
- Use proper ventilation and personal protective equipment (PPE) such as gloves and respirators.
- Store away from heat sources and oxidizing agents.

2. **Ethanol**

TWA:
- OSHA: Not explicitly regulated under TWA but considered hazardous due to flammability.
- STEL:
- Not specifically listed but must be handled with caution due to vapor flammability.

Health Hazards:
- Highly flammable liquid and vapor.
- Can cause eye irritation and respiratory discomfort upon inhalation.
- Safety Measures:
- Store in tightly sealed containers away from ignition sources.
- Handle in well-ventilated areas to minimize vapor accumulation.

3. **Sodium Hydroxide (NaOH)**

- TWA:
- OSHA: Ceiling limit of 2 mg/m^3 for workplace air concentration.

Health Hazards:

- Corrosive substance that can cause severe skin burns and eye damage.
- Inhalation of aerosols or dust can irritate the respiratory tract.

Safety Measures:

- Use chemical-resistant gloves, goggles, and protective clothing.
- Ensure proper ventilation during handling.

4. **Potassium Carbonate (K_2CO_3)**

Exposure Limits:

- No specific TWA or STEL established, but it is known to be an irritant.

Health Hazards:

- Can cause irritation to the skin, eyes, and respiratory system upon contact or inhalation.

Safety Measures:

- Handle with gloves and protective eyewear.
- Neutralize with acid before disposal.

5. **Catalyst Waste (TBAI)**

Exposure Limits:

- Specific limits are not established; however, it should be treated as hazardous waste due to its chemical properties.

Health Hazards:

- May cause irritation upon skin contact or inhalation of dust/fumes.

Safety Measures:

- Use PPE during handling and ensure proper containment.
- General Safety Guidelines for Handling Chemicals

Short-Term Exposure Limit (STEL):

- Exposures at STEL must not exceed a duration of more than 15 minutes at a time.
- A minimum interval of one hour should separate successive exposures at STEL levels.
- No more than four STEL exposures should occur within a single workday.

Ventilation:

- Ensure adequate ventilation in areas where chemicals are handled to prevent vapor accumulation.

Storage:
- Store chemicals in designated areas away from incompatible substances such as oxidizers or heat sources.

Spill Management:
- Use absorbents for spills and dispose of them as hazardous waste according to local regulations.

Personal Protective Equipment (PPE):
- Wear appropriate PPE such as gloves, goggles, face shields, and respirators based on the chemical being handled.
- By adhering to these exposure limits and safety measures, risks associated with handling hazardous chemicals during Fluroxypyr production can be minimized effectively.

References

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List of contributors

Vishal Raj (231163)

- Waste Generation and Quantities (Part a):
  - Listed the waste streams generated during Fluroxypyr production.
  - Calculated quantities of waste such as unreacted 4-Amino, Ethyl Glycolate, water, excess K_2CO_3, TBAI, hydrated $Na_2SO_4 \cdot 10H_2O$, ethanol, and NaCl.
- Regulations for Waste Materials (Part b):
  - Researched and explained regulations for hazardous waste disposal (e.g., Toluene, Ethanol, Sodium Hydroxide).
  - Detailed permissible exposure limits (PEL) and short-term exposure limits (STEL) for environmental disposal.
- Safety Concerns and Exposure Limits (Part d):
  - Highlighted safety concerns for chemicals like Toluene, Ethanol, Sodium Hydroxide, Potassium Carbonate, and TBAI.
  - Provided exposure limits (TWA for 8 hours and STEL for 15 minutes) and safety measures.
- EQ-factor calculation

Chandan Achary (230319)

- Treatment Procedure for Zero Liquid Discharge Plant with Block Diagram (Part c):
  - Designed and explained the ZLD system process flow in detail.
  - Created a block diagram showing pre-treatment, membrane treatment, thermal evaporation, crystallization, and solid waste management stages.
- Detailed Explanation of Waste Treatment:
  - Elaborated on recovery processes for catalysts like K_2CO_3 and TBAI.
  - Described methods for solid waste disposal and water recovery using multi-effect evaporators and crystallizers.
- Atom economy and E-factor calculation .
- Final Report Formatting:
  - Organized the entire report structure with clear headings for each section.
  - Ensured calculations were accurate and balanced in mass balance tables.

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