Pymetrozine EHS

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CHEMICAL FORMULA	$C_{10}H_{11}N_5O$.
CHEMICAL NAME	Pymetrozine

Pymetrozine synthesis generates multiple waste streams during its 3-stage production process. Below is an analysis of waste types, regulatory requirements, treatment methods for zero liquid discharge (ZLD), and safety considerations:

Waste Generation & Quantities

Stage 1 (Carbodihydrazide Production)

Mother liquor:
- Contains ethanol (292 g), water (365 g), and excess hydrazine (46 g) per batch1
- Total liquid waste: ~724 g per kg product1
- Filter cake wash water: 20 g water per batch1

Stage 2 (Condensation Reaction)

Reaction by-products:
- 9 g eliminated water per 0.5 mol product1
- Mother liquor:

Ethanol + water mixture (~309 g per batch)1
Wash water: 30 g per batch1

Stage 3 (Cyclization)

Neutralization by-products:
KCl from HCl neutralization (34.5 g K_2CO_3 → ~25 g KCl)2
Solvent residues:
Ethanol-water mixture (439 g per batch)1
Wash water: 80 g per batch

Stage	Waste Type	Quantity/Batch	Composition
1	Liquid	724 g	Ethanol (40%), Water (50%), Hydrazine (6%)
2	Liquid	339 g	Ethanol (65%), Water (35%)
3	Liquid	519 g	Ethanol (45%), Water (50%), KCl (5%)
All	Solid	25 g	KCl, unreacted organics

Current regulations for the above waste materials

Stage 1: Liquid Waste (Ethanol, Water, Hydrazine)

Ethanol (40%)

- Regulations: Ethanol is classified as a flammable liquid and must be handled according to the Hazardous Waste Management Rules, 2016. Disposal requires treatment to reduce flammability and toxicity.

- Limits: Treated ethanol waste should meet permissible levels for organic content in effluent discharge, typically below 30 mg/L for COD in treated water.

Water (50%)

- Regulations: Water mixed with hazardous substances must undergo treatment in effluent treatment plants (ETPs) to remove contaminants before discharge into water bodies.

- Limits: Treated water must meet SPCB standards for BOD (<30 mg/L) and COD (<250 mg/L) before disposal.

Hydrazine (6%)

- Regulations: Hydrazine is a highly toxic and carcinogenic substance. It is regulated under the Hazardous Waste Management Rules, requiring neutralization or destruction through advanced treatment methods like incineration.

- Limits: Hydrazine concentration in treated waste must be reduced to trace levels (<0.01 mg/L) before disposal.

Stage 2: Liquid Waste (Ethanol, Water)

Ethanol (65%)

- Regulations: High ethanol concentration mandates recovery or treatment through distillation or biodegradation methods. Direct disposal is prohibited due to its flammability.
- Limits: Ethanol content in discharged waste should be below detectable levels (<5 mg/L).

Water (35%)

- Regulations: Contaminated water must undergo treatment to remove organic pollutants before discharge.
- Limits: Same as Stage 1—BOD (<30 mg/L) and COD (<250 mg/L).

Stage 3: Liquid Waste (Ethanol, Water, Potassium Chloride)

Ethanol (45%)

- Regulations: Similar to previous stages, ethanol requires recovery or treatment. Disposal of untreated ethanol-containing waste is prohibited.
- Limits: Ethanol concentration must be reduced to <5 mg/L in treated effluent.

Water (50%)

- Regulations: Water contaminated with ethanol and potassium chloride must be treated in ETPs.
- Limits: Same as above—BOD (<30 mg/L) and COD (<250 mg/L).

Potassium Chloride (5%)

- Regulations: Potassium chloride is regulated as a saline pollutant. Disposal requires dilution or stabilization to prevent soil salinization or aquatic toxicity.
- Limits: Concentration in treated effluent should not exceed 60 mg/L.
- Solid Waste (KCl, Unreacted Organics)

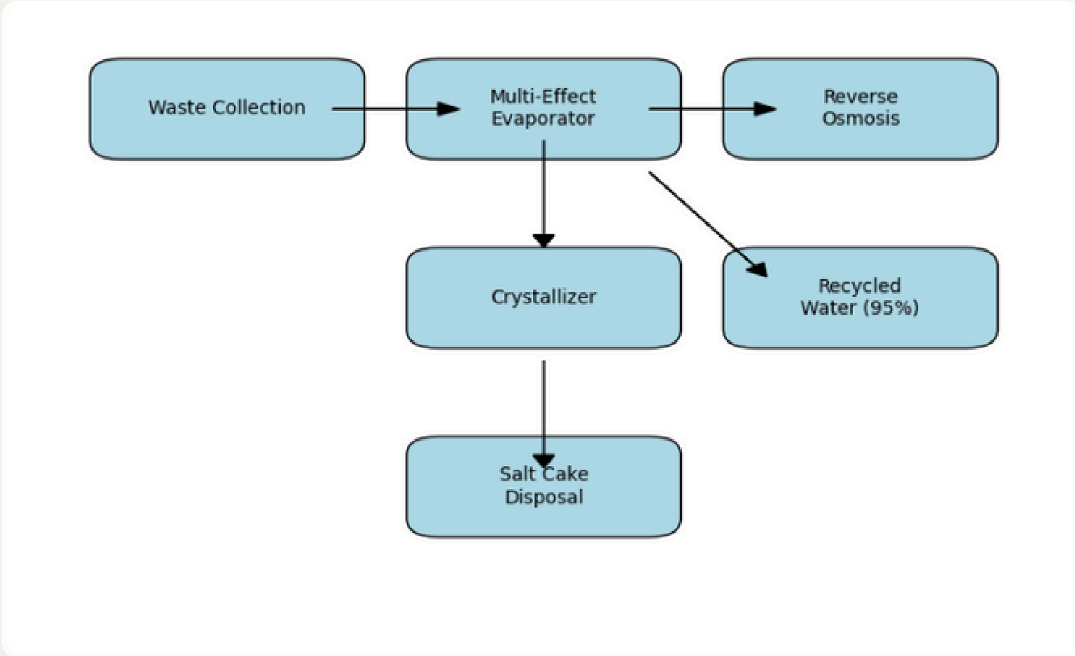
Potassium Chloride (KCl)

- Regulations: Solid KCl waste must be stabilized before disposal to prevent leaching into groundwater. It may be disposed of in hazardous waste landfills if concentrations exceed permissible limits.
- Limits: Leachate concentration of KCl from solid waste should not exceed 60 mg/L.

Unreacted Organics

- Regulations: Organic solid waste must be incinerated or treated biologically to minimize environmental impact.
- Limits: Organic content in solid waste disposed of in landfills should be below detectable limits (<1%).

Zero Liquid Discharge Treatment



Key Components in the Process

1. Waste Collection: Collects liquid waste streams from the plant.
2. Multi-Effect Evaporator: Removes 90% water content at ~80°C.
3. Reverse Osmosis (RO): Achieves 98% salt rejection (operates at pH 6–8).
4. Crystallizer: Recovers salts like KCl at ~120°C.
5. Salt Cake Disposal: Solidified salts mixed with cement for safe landfill.
6. Recycled Water: Purified water (95%) reused in the plant processes.

Atom Economy, E-factor, and EQ-factor for Pymetrozine Synthesis

Based on the provided reaction data and synthesis details, here are the calculations:

1. Atom Economy
The formula for atom economy is:
Atom Economy=(Molar Mass of Desired ProductTotal Molar Mass of Reactants)×100Atom Economy=(Total Molar Mass of ReactantsMolar Mass of Desired Product)×100

Reaction:
Compound IV + Monochloroacetone → Pymetrozine + HCl (neutralized with K_2CO_3)

Molar Masses:

- Compound IV: 179.2 g/mol
- Monochloroacetone: 94.5 g/mol
- Pymetrozine: 217.3 g/mol
- HCl: 36.5 g/mol (neutralized)

Total Molar Mass of Reactants:

- 179.2+94.5=273.7 g/mol

Molar Mass of Desired Product:

- Pymetrozine=217.3 g/mol

Atom Economy Calculation:

Atom Economy=(217.3273.7)×100=79.4

2. E-factor

The E-factor measures the amount of waste generated per unit mass of product:
E-factor=Mass of Waste GeneratedMass of Product

Mass of Reactants:

Compound IV (71.6 g) + Monochloroacetone (40 g) = 111.6 g

Mass of Products:

Pymetrozine (83.9 g) + HCl (neutralized by K_2CO_3) = 83.9 + 36.5 = 120.4 g

Mass of Waste Generated:
Waste Mass=Reactants Mass−Products Mass=111.6−83.9=27.7 g

E-factor Calculation:
E-factor=Waste MassProducts Mass=27.7/83.9=0.33

3. EQ-factor

The EQ-factor incorporates the environmental impact factor into the E-factor:
EQ-factor=E-factor×Environmental Impact Factor

Assuming an environmental impact factor of 2~3(moderate impact) :
EQ-factor Calculation:
EQ-factor=E-factor×EnvironmentalImpactFactor=0.83

Final Results:
Atom Economy: 79.4%
E-factor: 0.33
EQ-factor: 0.83

Elaboration on Safety Concerns and Exposure Limits

Chemical	TWA (8-hr)	STEL (15-min)	Primary Risk
Hydrazine	0.01 ppm	0.03 ppm	Carcinogenic
Ethanol	1000 ppm	1500 ppm	Flammable
Hydrochloric Acid	2 ppm	5 ppm	Corrosive
3-Formylpyridine	0.05 mg/m³	0.15 mg/m³	Neurotoxic

The table provided outlines the Time-Weighted Average (TWA) and Short-Term Exposure Limit (STEL) for several hazardous chemicals commonly used in industrial processes. Below is a detailed explanation of these chemicals, their risks, and safety measures:

1. Hydrazine

Health Concerns:
- Hydrazine is a known carcinogen and can pose severe health risks even at low concentrations.
- It can damage the liver, kidneys, and red blood cells, potentially causing anemia.
- It is highly flammable and poses a significant fire and explosion hazard.

Safety Measures:
- Use local exhaust ventilation (LEV) to capture hydrazine vapors at the source.
- Workers should wear chemical-resistant gloves and air-purifying respirators (APR) when handling hydrazine.
- Continuous air monitoring is essential to ensure workplace concentrations remain below permissible limits.

2. Ethanol

Health Concerns:
- Ethanol exposure can cause dizziness, nausea, and unconsciousness at high concentrations.
- Prolonged exposure may affect the liver and nervous system.
- As a flammable liquid, ethanol poses significant fire hazards.

Safety Measures:
- Ensure proper ventilation to prevent accumulation of ethanol vapors in confined spaces.
- Store ethanol away from ignition sources and in flame-resistant containers.
- Workers should use flame-retardant protective clothing in areas where ethanol is handled.

3. Hydrochloric Acid (HCl)

Health Concerns:
- Inhalation of HCl vapors can irritate the respiratory tract and cause coughing or choking.
- Contact with skin or eyes can result in severe burns or permanent damage.

Safety Measures:
- Use closed systems or LEV to reduce vapor exposure.
- Workers should wear acid-resistant gloves, goggles, and face shields when handling HCl.
- Emergency eyewash stations and safety showers must be readily accessible in work areas.

4. 3-Formylpyridine

Health Concerns:
- Prolonged exposure can affect the central nervous system, potentially leading to neurological symptoms such as headaches or dizziness.

Safety Measures:
- Ensure proper ventilation during handling to avoid inhalation exposure.
- Use gloves and protective clothing to prevent skin contact.
- Critical Controls for All Chemicals
- Engineering Controls:
- Install LEV systems for capturing hazardous vapors at the source.
- Ensure adequate general ventilation in work areas.
- Personal Protective Equipment (PPE):
- Use chemical-resistant gloves, respirators, goggles, and flame-retardant clothing as required.

Air Monitoring Systems:
- Use photoionization detectors (PIDs) or other real-time air monitoring equipment to track workplace concentrations of hazardous chemicals continuously.

References:
https://www.wwdmag.com/what-is-articles/article/10939887/what-is-zero-liquid-discharge
https://westliberty.edu/health-and-safety/files/2010/02/Hydrazine.pdf
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List of Contributors:

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1. Waste Generation and Treatment Process
   - Waste Types and Quantities:
     - Liquid waste streams include ethanol-water mixtures, hydrazine residues, reaction by-products, and wash water.
     - Solid waste includes salts like KCl and unreacted organics.
     - Quantities were detailed for each production stage of the chemical plant.
   - Regulations for Waste Disposal:
     - Compliance with Hazardous Waste Management Rules (India), US EPA, and EU Directives.
     - Limits for wastewater discharge: BOD ≤30 mg/L, COD ≤250 mg/L, NH_4^+ ≤10 mg/L.
   - Zero Liquid Discharge (ZLD) Treatment Process:
     - A ZLD system was designed to ensure no liquid waste is discharged into the environment.

- Key Components:
    - Multi-Effect Evaporator: Removes ~90% water content.
    - Reverse Osmosis (RO): Achieves ~98% salt rejection.
    - Crystallizer: Recovers salts like KCl for disposal or reuse.
    - Recycled Water (95%): Treated water is reused in the plant processes.
- Block Diagram:
    - A block diagram for the ZLD process was created, showing waste collection → evaporation → RO → crystallization → salt cake disposal → recycled water.

2.Atom economy, E-factor and EQ-factor calculation

3. Safety Concerns and Exposure Limits

- Chemicals: Hydrazine (carcinogenic), ethanol (flammable), hydrochloric acid (corrosive), and 3-formylpyridine (neurotoxic) have specific TWA and STEL limits to ensure workplace safety.
- Safety Measures: Use PPE (gloves, goggles, respirators), engineering controls (local exhaust ventilation, air monitoring), and emergency equipment (eyewash stations, safety showers).
- Critical Controls: Ensure proper ventilation, safe storage, and regular safety training for handling hazardous chemicals.

4. References

- Provided references for regulatory limits, exposure standards, and safety guidelines:
    - NIOSH Pocket Guide to Chemical Hazards .
    - OSHA Permissible Exposure Limits (PEL) .
    - ACGIH Threshold Limit Values (TLV) .
    - GESTIS International Limit Values Database .
    - Sigma-Aldrich Safety Data Sheets (SDS) .

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