Nature of Invention: Chemical molecule and synthesis route

Applicant: GreenovateX

Inventors: Navdeep

Chemical Formula: $C_{10}H_{19}O_6PS_2$

Chemical Name: Malathion

Chemical synthesis routes:

1. Direct Esterification of O,O-Dimethyl Phosphorodithioic Acid

Chemicals Required

1. O,O-Dimethyl Phosphorodithioic Acid (DMPA)Diethyl Maleate (DEM) – $C_2H_5O_2CCH{=}CHCO_2C_2H_5$
3. Sulfuric Acid (H_2SO_4) or p-Toluenesulfonic Acid
4. Toluene ($C_6H_5CH_3$) or Xylene (C_8H_{10})
5. Molecular Sieves (3Å or 4Å) or Anhydrous Sodium Sulfate (Na_2SO_4)
6. Sodium Carbonate (Na_2CO_3) or Sodium Hydroxide (NaOH)

Vessels Required

1. **Esterification Reactor (Glass-Lined or Stainless Steel Reactor with Acid Resistance)**
2. **Mixing Vessel**
3. **Separation Vessel (Decanter/Settler)**
4. **Filtration Unit (Vacuum Filter or Pressure Filter)**
5. **Distillation Column (Fractional Distillation Unit)**
6. **Product Storage Tank (HDPE or Stainless Steel with Antioxidant Lining)**
7. **Solvent Storage Tank**
8. **Waste Neutralization Tank**

Process analysis

1. Objective

To produce **Malathion ($C_{10}H_{19}O_6PS_2$)** using the **direct esterification of O,O-Dimethyl Phosphorodithioic Acid (DMPA)** with **Diethyl Maleate (DEM)** in the presence of catalysts, followed by purification.

2. Chemical Reaction

O,O-Dimethyl Phosphorodithioic Acid+Diethyl Maleate→Malathion+H2O

- **Reactants:**
  - O,O-Dimethyl Phosphorodithioic Acid (DMPA) → **$(CH_3O)_2PS_2H$**
  - Diethyl Maleate (DEM) → **$C_6H_{10}O_4$**
- **Products:**
  - Malathion → **$C_{10}H_{19}O_6PS_2$**
  - Water (byproduct)
- **Catalysts/Additives:**
  - **Sulfuric Acid (H_2SO_4)** or **p-Toluenesulfonic Acid (p-TSA)** as an acid catalyst.
  - **Sodium Hydroxide (NaOH)** for neutralization.

3. Reaction Conditions

Temperature	80-100°C
Pressure	Atmospheric or slight vacuum
Catalyst	Sulfuric Acid (H_2SO_4) / p-TSA
Reaction Time	2-4 hours
pH Control	NaOH neutralization (pH 7-8)

4. Process Flow

Step 1: Raw Material Preparation

- O,O-Dimethyl Phosphorodithioic Acid (DMPA) and Diethyl Maleate (DEM) are mixed in a **Mixing Vessel**.
- Catalyst (H_2SO_4 or p-TSA) is added to initiate the esterification reaction.

Step 2: Esterification Reaction

- The mixture is transferred to **Reactor 1**, where it is heated to **80-100°C** for 2-4 hours.
- Malathion forms along with **water as a byproduct**.

Step 3: Water Removal

- The reaction mixture is sent to a **Vacuum System**, which removes excess water to drive the reaction forward.

Step 4: Neutralization & pH Adjustment

- The crude product is treated with **NaOH or Na_2CO_3** in **Reactor 2** to neutralize residual acid.
- The pH is adjusted to **7-8** to prevent decomposition.

Step 5: Liquid-Liquid Extraction

- The mixture enters a **Liquid Extraction Column**, where **organic Malathion** is separated from the aqueous phase.
- Aqueous waste (salts and excess water) is removed.

Step 6: Filtration

- The organic phase undergoes **Pressure Filtration** to remove **impurities and solid residues** (NaCl and unreacted materials).

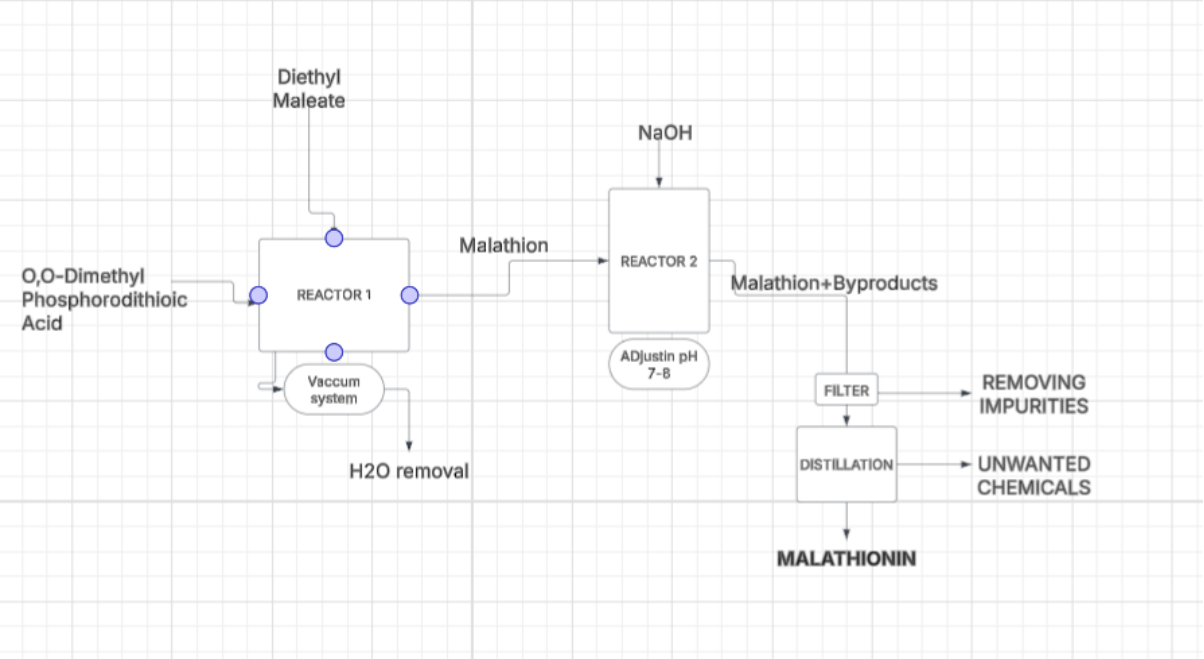
Step 7: Solvent Removal & Drying

- The filtered solution is sent to a **Vacuum Dryer or Distillation Column** to remove any residual solvents.
- This ensures **98%+ pure Malathion**.

Step 8: Storage & Stabilization

- The purified Malathion is stored in a **Storage Tank** with **stabilizers (e.g., antioxidants)** to prevent degradation.

5. Process Flow Diagram (PFD) Overview



Stage	Equipment Used	Output
Raw Material Prep	Mixing Vessel	DMPA + DEM Mixture
Esterification	Reactor 1 (80-100°C)	Crude Malathion + Water
Water Removal	Vacuum System	Malathion + less water
Neutralization	Reactor 2 (pH 7-8)	Neutralized Malathion
Extraction	Liquid Extraction Column	Organic Malathion, Aqueous Waste
Filtration	Pressure Filter	Purified Malathion Solution
Drying	Vacuum Dryer	98%+ Pure Malathion
Storage	Storage Tank	Final Malathion with Stabilizers

2. Malathion Production via Thiophosphorylation of Diethyl Fumarate/Diethyl Maleate

Chemicals Required

- **Phosphorus Pentasulfide (P_2S_5)**
- **Methanol (CH_3OH)**
- **Diethyl Maleate (DEM) or Diethyl Fumarate (DEF)**
- **Sulfuric Acid (H_2SO_4) or Sodium Hydroxide (NaOH)**
- **Tertiary Amines (e.g., Triethylamine, Pyridine)**
- **Toluene, Dichloromethane (DCM), or Hexane**
- **Water (Deionized or Distilled)**
- **Sodium Bicarbonate ($NaHCO_3$) or Sodium Hydroxide (NaOH)**

Vessels Required

- **Storage Tanks**
- **Agitated Feed Tanks**
- **Jacketed Stirred Tank Reactor**
- **Reflux Condenser**
- **Heat Exchanger (Shell & Tube or Plate Type)**
- **Vacuum System (Rotary Vacuum Pump)**
- **Nutsche Filter / Pressure Filter**
- **Liquid-Liquid Extraction Column**
- **Thin Film Evaporator / Falling Film Evaporator**
- **Spray Dryer / Vacuum Dryer**

Process Analysis

1. Objective

To produce Malathion through the thiophosphorylation of Diethyl Fumarate/Diethyl Maleate using O,O-dimethyldithiophosphoric acid.

2. Chemical Reactions

1. **Synthesis of O,O-Dimethyl Dithiophosphoric Acid**:

$$P2S5+4CH3OH \rightarrow 2(CH3O)2P(S)SH+H2S$$

2. **Thiophosphorylation Reaction (Formation of Malathion):**
$$(C2H5O2C)CH=CH(COOC2H5)+(CH3O)2PS2H \rightarrow Malathion+Byproducts$$

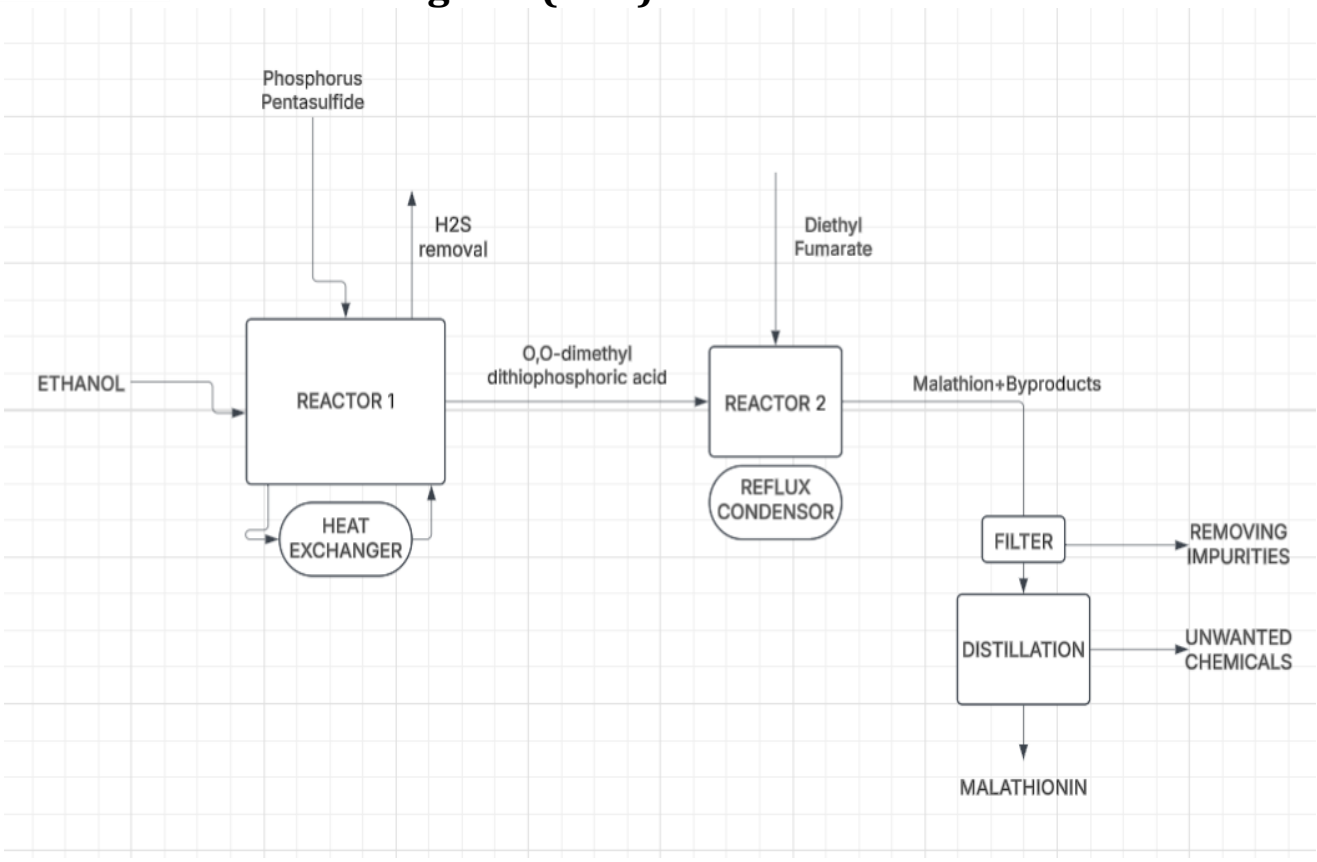
3. Reaction Conditions

- **Synthesis of O,O-Dimethyl Dithiophosphoric Acid**:
  - **Temperature**: 50-60°C.
  - **Reaction Time**: 1-2 hours.
  - **Pressure**: Atmospheric.
  - **Stirring**: Continuous.
- **Thiophosphorylation Reaction**:
  - **Temperature**: 50-80°C.
  - **Pressure**: Atmospheric or slight vacuum.
  - **Reaction Time**: 3-6 hours.
  - **Catalyst (if used)**: Acidic (H_2SO_4) or Basic (NaOH).

4. Process Flow

1. **Raw Material Preparation & Handling**:
   a. Store and transfer reactants under controlled conditions.
   b. Required materials: P_2S_5, CH_3OH, DEM/DEF, catalysts (if used), and solvents.
2. **Preparation of O,O-Dimethyl Dithiophosphoric Acid**:
   a. React P_2S_5 with CH_3OH to form dimethyl dithiophosphoric acid.
   b. Conditions: 50-60°C, 1-2 hours, atmospheric pressure.
3. **Thiophosphorylation Reaction (Formation of Malathion)**:
   a. React O,O-dimethyl dithiophosphoric acid with DEM/DEF.
   b. Conditions: 50-80°C, 3-6 hours, atmospheric or slight vacuum.
4. **Filtration & Solvent Removal**:
   a. Remove solid impurities via filtration.
   b. Evaporate solvent using a thin-film evaporator or distillation.
   c. Neutralize if necessary.
5. **Drying & Final Product Storage**:
   a. Dry the product under vacuum conditions.
   b. Store Malathion in pure liquid or powder form.

5. Process Flow Diagram (PFD)



Stage	Equipment Used	Output
Raw Material Prep	Agitated Feed Tanks	P_2S_5 + CH_3OH + DEM/DEF Mixture
Synthesis of Dithiophosphoric Acid	Jacketed Stirred Tank Reactor	O,O-Dimethyl Dithiophosphoric Acid
Thiophosphorylation	Jacketed Stirred Tank Reactor	Crude Malathion
Filtration & Solvent Removal	Nutsche Filter / Pressure Filter & Thin Film Evaporator	Purified Malathion Solution
Drying	Vacuum Dryer	Pure Malathion
Storage	Storage Tanks	Final Malathion Product

Reasons due to which The Direct Esterification of O,O-Dimethyl Phosphorodithioic Acid is a more efficient route for Malathion production compared to the Thiophosphorylation of Diethyl Fumarate.

- Direct Esterification of O,O-Dimethyl Phosphorodithioic Acid gives higher yield (~98%) and is more efficient.
- Thiophosphorylation of Diethyl Fumarate is safer as it avoids $POCl_3$ and NaCN.
- Direct Esterification has faster reaction time and simpler purification steps.
- Thiophosphorylation operates under milder conditions (50-80°C) but has lower yield (~92-95%).
- Direct Esterification requires strict anhydrous conditions, as reactants are moisture-sensitive.
- Thiophosphorylation involves more reaction steps, leading to higher operational costs.
- Direct Esterification is preferred for industrial production due to better efficiency and cost-effectiveness.
- Thiophosphorylation is a viable alternative when safety and environmental factors are a priority.

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List the contributions of each author:Navdeep

- Designed and implemented a chemical synthesis route for the production of Malathion, including raw material selection, process design, and optimization of key stages such as esterification, purification, and drying.
- Explored an alternative way to produce malathion through the thiophosphorylation of Diethyl Fumarate/Diethyl Maleate using O,O-dimethyldithiophosphoric acid.
- Figured out which process is better and its reasoning which can be more friendly for company and production

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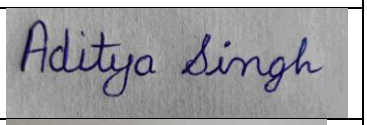
Aditya Singh	230079	
Navdeep	230683