Nature of Invention: Process design

Applicant: GreenovateX

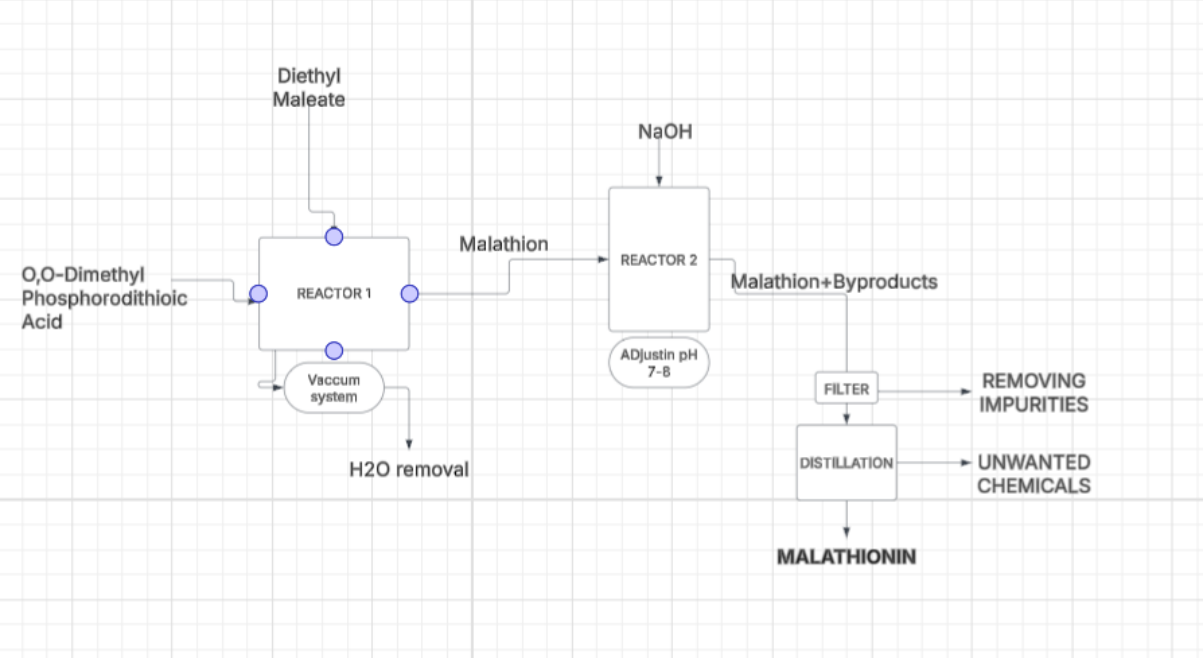
Inventors: Priyanshu Kumar Choudhary, Sanjeeta Singh

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

Chemical Name: Malathion

Process Title : Production of Malathion from Direct Esterification of O,O-Dimethyl Phosphorodithioic Acid

Process flow diagram –



Process Description:

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)

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

Material balance :

For the reaction taking part in reactor we have to prepare **O,O-dimethyldithiophosphoric acid (OODMDTPA)**:

1. Reaction involved in the formation of **O,O- dimethyldithiophosphoric acid (OODMDTPA)**: -

$P2S5+4CH3OH \rightarrow 2OODMDTPA+H2S\uparrow$

Reaction in Reactor 1 (Esterification Step)

$C_8H_{12}O_4+(CH_3O)_2PS_2H \rightarrow C_{10}H_{19}O_6PS_2+H_2O$

- At controlled temperature(80–100°C) the reaction takes about 7 hours of time

Going step by step,

- We have **Diethyl Maleate (DEM) ($C_8H_{12}O_4$)** and

  O,O-Dimethyl Phosphorodithioic Acid (DMDTPA) ($(CH_3O)_2PS_2H$)

  as our reactant,

  And **Malathion ($C_{10}H_{19}O_6PS_2$)** as our main product

  And **Water (H_2O)** as our By-product (the by product is removed by vacuum system)

We are having some input data for the reactor. After the reaction we have to keep in mind that pH also play a vital role in efficient production.

Here are some inputs on daily basis-

We are assuming 1000kg on daily basis

Component	Molecular weight (g/mol)	Mass ratio	Daily requirement(kg/day)
Diethyl Maleate (DEM)	172	172/330	512.2
DMDTPA	176	176/330	533.3
Water (By-product, removed)	18	18/330	54.5(kg removed)
NaOH (for pH adjustment)	40		50

- For mass ratio the denominator 330 is the molar mass of malathion.
- To produce 1000kg of malathion we require - 512.3kg of DEM, 533.3kg of DMDTPA, 54.4kg of and 50kg of NaOH.
- We have not calculated the mass ratio for NaOH as it is not taking part in reaction it is for pH adjustment only.

Parameters for the reactor-

- Temperature: - 80–100°C
- Pressure: - 2 – 3 bar
- Volume: - 1-2 m^3

Here total mass input = 512.2 + 513.3 + 50

= 1075.5

Now below is the table for output in from reactor –

Component	Output per day (in kg)	What to do next
Malathion (Main Product)	1000	Sent for packaging
Water (By-product, removed)	54.5	Discarded or removed

Sodium Salts & Impurities	50.0	Removed in filtration
Unwanted Chemicals (Distillation Waste)	30.0	Recycled or disposed

Total output per day = 1000 kg Malathion +104.5 kg of by-products and 30 kg of waste for recycling

- See during all these reactions taking place in the reactor we have to adjust the pH which we have adjusted by adding NaOH
- The pH is adjusted to 7 – 8:

pH Adjustment & Neutralization (Side Reaction) :

$H_3PO_4+NaOH \rightarrow NaH_2PO_4+H_2O$

Why pH adjustment?

- Malathion contains residual phosphorodithioic acid-based impurities, which are neutralized using **sodium hydroxide (NaOH)** to adjust the pH to **7-8**.

By-products: Sodium salts (NaH_2PO_4, Na_2SO_4), removed during purification.

For pH adjustment in reactor:

- Temperature range: 30–40°C
- Volume nearly 4 to 5 m^3

After pH adjustment the products are now filtered in filtration column.

- In filtration column removal of solid by-products takes place.
- Capacity of filtration column is around 250kg/hr.

After filtration the malathion is still unpure, there are some impurities remained in the product.

To remove these impurities, we have to pass the product through distillation column as shown in the figure.

- Generally, it is packed column.
- Height about 5m.
- Diameter about 1m.

Conclusion & Recommendations

- high-purity Malathion (~95%) is produced through esterification & purification.
- By-products like water & sodium salts can be recycled or sold, improving sustainability.
- This balance ensures **efficient raw material utilization** and **minimal waste generation** at the **industrial level**.

economic analysis:

Raw material cost:

Raw material	Quantity required(kg/day)	Cost per kg (₹)	Total Cost per Day (₹)
Diethyl Maleate (DEM)	512.2	380	1,94,636
DMDTPA	513.3	420	2,23,986
NaOH	50	60	3,000
Total Raw Material Cost	-	-	₹4,21,622

Utilities cost:

Utility	Consumption per day	Cost per Unit (₹)	Total Cost per Day (₹)
Electricity	1,420 kWh	8/kWh	11,360
Steam & Labour	-	-	21,750
Cooling Water	-	-	300
Compressed Air	-	-	300
Effluent Treatment & Waste Disposal	-	-	250
Total Utilities Cost	-	-	₹33,960

Total Production Cost & Per Kg Cost:

Description	Amount (₹)
Total Raw Material Cost	4,21,622
Total Utilities Cost	33,960
Total Cost per Day	₹4,55,582
Cost per kg of Malathion Production	₹455.58

Revenue & Profit Calculation:

Description	Amount (₹)
Market Price of Malathion (including GST)	₹1,420 per kg
Total Revenue per Day (1,000 kg)	₹14,20,000
Total Profit per Day	₹14,20,000 - ₹4,55,582 = ₹9,64,418

.

Capital cost (only for the reactor):

example:

Equipment	Design Capacity (L)	No. of units	Cost/unit (₹for year 2014)	Total Cost (₹for year 2014)
Reactor 1 (Jacketed reactor, agitated, stainless steel, atm. pressure)	1500	1	₹83,93,723.56	₹83,93,723.56
Reactor 2 (Jacketed reactor, agitated, stainless steel, atm. pressure)	1500	1	₹83,93,723.56	₹83,93,723.56

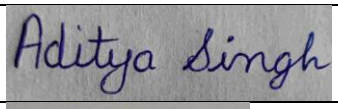
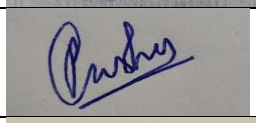
References: Provide reference for a research paper or an actual patent.

1. http://www.matche.com/equipcost/Reactor.html

List the contributions of each author:

- Priyanshu Kumar Choudhary: Material Balance and Reactor costing analysis.
- Sanjeeta Singh : Block diagram

Sign the pdf and upload.

Name	Roll No	Signature
CEO Name	Aditya Singh	
First author Name	Priyanshu Kumar Choudhary	
Second author Name (if any)	Sanjeeta Singh