Technical Team

Applicant: VortexChem

Inventors: P. Shruti Sekhar , Shantanu Prakash

Chemical Formula: $C_{28}H_{22}Cl_2FNO_3$

Chemical Name: Flumethrin

Cyano(4-fluoro-3-phenoxyphenyl)methyl 3-[(Z)-2-chloro-2-(4-chlorophenyl)ethenyl]-2,2-dimethylcyclopropane-1-carboxylate

Process Title: Industrial Production of Flumethrin

Raw materials and chemicals required: 4-Fluoro-3-Phenoxybenzaldehyde, Bayticol P Acid Chloride, Sodium Cyanide (NaCN), Thionyl Chloride, Toluene, DMF, NaOH, HCl, SO_2, Water.

Process Description:

Flumethrin is synthesized through a multi-step reaction involving chlorination, cyanation, and purification.

1. Stirred Tank Reactor-1: Bayticol P Acid reacts with Thionyl Chloride in Toluene and DMF to form the acid chloride. Water is added to control excess $SOCl_2$.

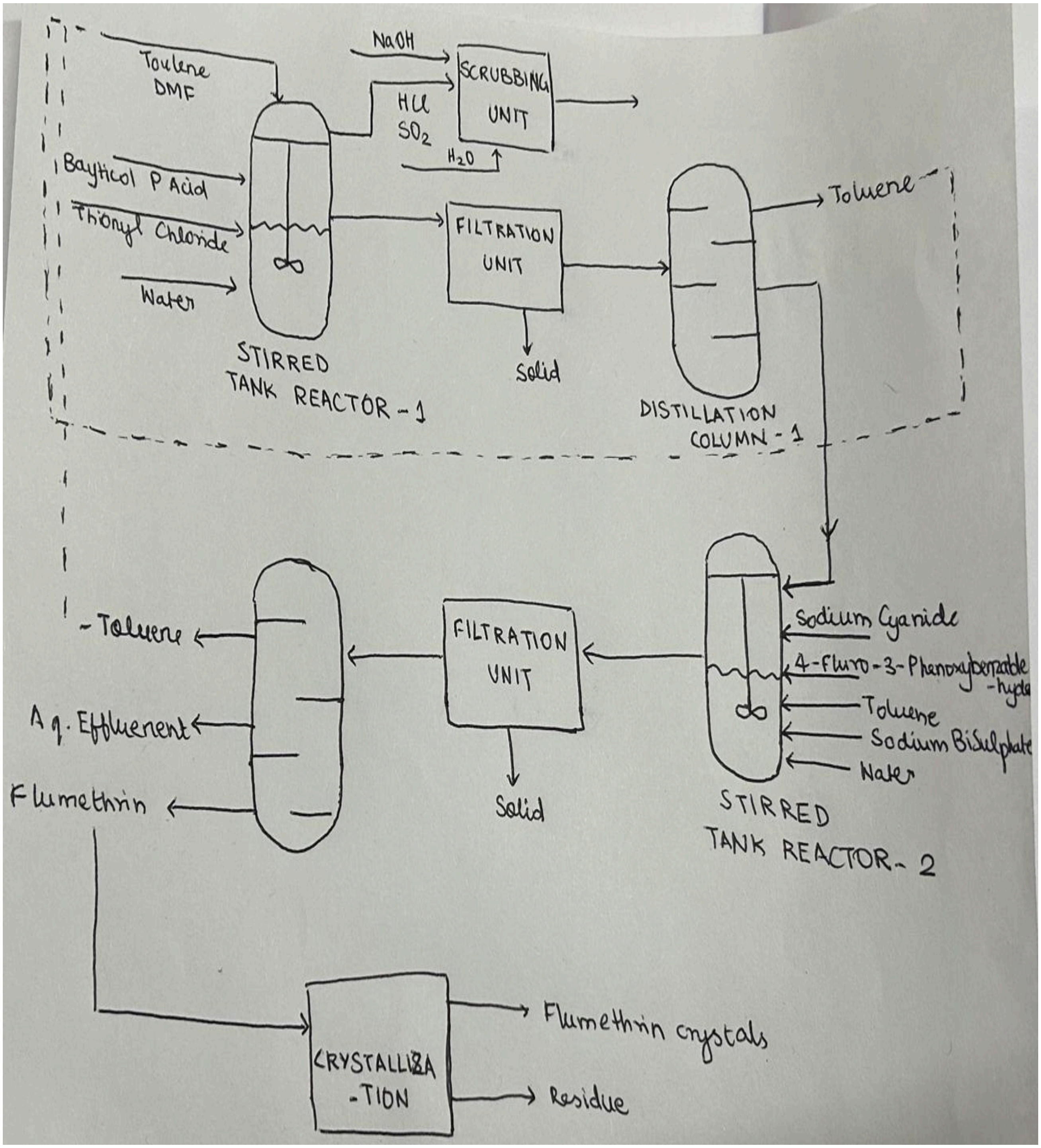
2. Scrubbing Unit: Acidic gases (SO_2, HCl) are neutralized using NaOH to prevent environmental release.

3. Filtration & Distillation: Solid impurities are removed, and Toluene is recovered for reuse.

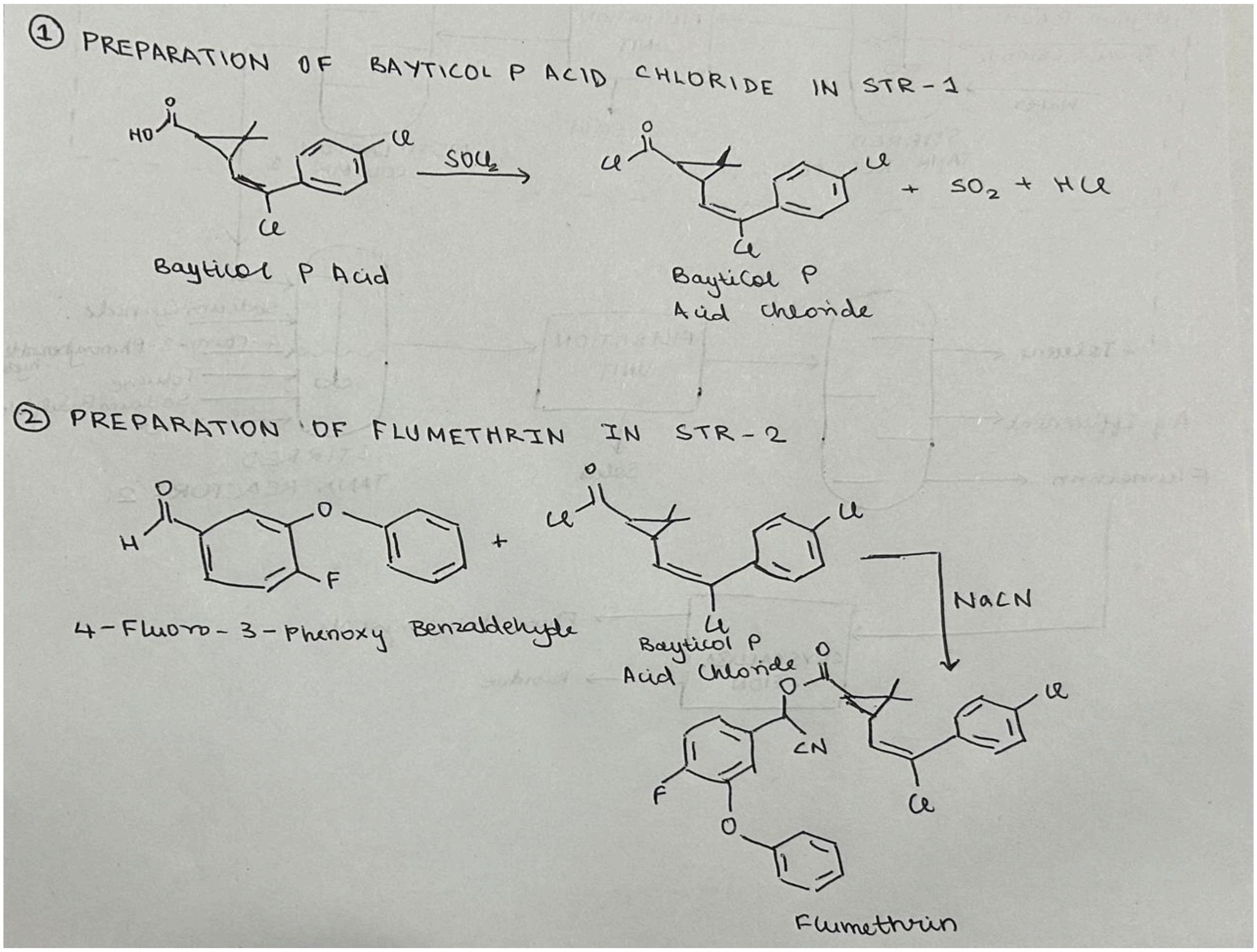
4. Stirred Tank Reactor-2: The acid chloride reacts with NaCN and 4-Fluoro-3-Phenoxybenzaldehyde in Toluene to form Flumethrin.

5. Final Purification: Filtration removes residual solids, and the purified product undergoes crystallization and drying. The final product purity is **~ 98%** .

Process Flowsheet for the production of Flumethrin :



Reactions Involved:



Reaction 1 :

Reactor Type : Stirred Tank Reactor

Operating Temperature : 80 C

Product Yield : 95 %

Reaction 2 :

Reactor Type : Stirred Tank Reactor

Operating Temperature : 60 C

Product Yield : 90 %

Material Balance:

Basis : 1000 kg Flumethrin / day

Assuming a yield of 90% for Reaction - 2,

Let 'x' be the flow rate (molar) of Flumethrin exiting STR - 2,

MW (Flumethrin) = 510.4 g

$$x = \frac{1000\ kg}{MW_{Flumethrin}}$$

$$x = \frac{1000\ kg}{510.4\ g} = 1.96\ kmol/day$$

Required 4F3P × 0.9 (yield) = 1.96 kmol/day

∴ 4 - Fluoro - 3 - Phenoxy Benzaldehyde = 2.177 kmol/day ≅ 2.2 kmol/day

Required Bayticol P - Acid Chloride = 2.2 kmol/day

Mass of 4F3P (input to STR - 2) = 2.2 × 216.2 kg/day = 471 kg/day

MW (4F3P) = 216.2 g

Mass of Bayticol P-Acid chloride (input to STR-2) = 2.2 × 303.6 kg/day = 661 kg/day

MW (Bayticol P Acid Chloride) = 303.6 g

Mass of NaCN (input to STR-2) = 2.2 × 49 kg/day = 108 kg/day

Assuming a yield of 95% for Reaction - 1,

Required Bayticol P - Acid × 0.95 (yield) = 2.2 kmol/day

Req Bayticol P- Acid = 2.31 kmol/day

MW (Bayticol P- Acid) = 283.2 g

Mass of Bayticol P- Acid (Input to STR - 1) = 653 kg/day

Req $SOCl_2$ = 2.31 kmol/h

Mass of $SOCl_2$ (input to STR-1) = 2.31 × 118.97 kg/h = 276 kg/day

MW ($SOCl_2$) = 118.97 g

MASS BALANCE AROUND STR-1

Mass of HCl (Output from STR-1) = 2.2 × 36.5 kg/h = 80 kg/day

[Stoichiometric ratio of Baticol P Acid Chloride, HCl and SO_2 is 1:1:1]

Mass of SO_2 (Output from STR-1) = 2.2 × 64 kg/h = 141 kg/day

Mass of unreacted reactants = 653 + 276 − 80 − 141 − 661 $\frac{kg}{day}$ = 47 kg/day

MASS BALANCE AROUND SCRUBBER

Scrubbing reactions :

$HCl + NaOH \longrightarrow NaCl + H_2O$

$SO_2 + NaOH \longrightarrow NaHSO_3$

NaOH req = 2.2 + 2.2 kmol/day = 4.4 kmol/day

Mass of NaOH (input to scrubber) = 4.4 × 40 kg/day = 176 kg/day

∴ Mass of Neutralized products = ~~176~~ (141 + 80 + 176) $\frac{kg}{day}$ = ~~45~~ 397 kg/day

PER DAY MATERIAL BALANCE :

INPUTS	MASS	OUTPUTS	MASS
Bayticol P Acid	653 kg	Bayticol P Acid chloride	661 kg
Thionyl Chloride	276 kg	Neutralized products	397 kg
NaOH	176 kg	Unreacted reactants	47 kg
TOTAL	1105 kg	TOTAL	1105 kg

Hence, Material balance around unit operations STR-1 and Scrubber is shown.

MASS BALANCE AROUND STR-2

Stoichiometric

Mass of unreacted reactants = − Mass of Flumethrin + Mass of input reactants

= −1000 + (471 + 661 + 108) kg/day

Mass of unreacted reactants = 240 kg/day

INPUTS	MASS	OUTPUTS	MASS
Bayticol P Acid Chloride	661 kg	Flumethrin	1000 kg
Sodium Cyanide	108 kg	Unreacted reactants	240 kg
4F3P	471 kg		
TOTAL	1240 kg	TOTAL	1240 kg

Hence, Material balance around unit operation STR-2 is shown.

The previous calculations were based on stoichiometric assumptions. However, in large-scale industrial production, inefficiencies such as side reactions, incomplete conversions, and material losses must be considered. Based on data from existing patents and research papers, the actual material balance accounts for these factors, ensuring a more realistic estimation of reactant consumption and product yield. These adjustments help optimize raw material usage, minimize waste, and improve overall process efficiency.

Additionally, the market analysis and other teams have relied on this industrial material balance for their assessments, as it provides a more accurate representation of real-world production conditions compared to theoretical stoichiometric data.

Step-1: Preparation of Bayticol P acid chloride

Material Balance:

Input	kg		Output	Kg
Bayticol P Acid	590		Bayticol P Acid Chloride	627
Thionyl Chloride	277		Toluene with product to stage 2	941
Toluene	1805		HCl gas	76
DMF	1		SO2 gas	130
Water	1544	→	Rec. Toluene	835
Sodium hydroxide	69		Aq. Effluent	1648
			Residue	29
	4286			4286

Step-2: Preparation of Flumethrin

Material Balance:

Input	kg		Output	Kg
Bayticol P Acid	627		Flumethrin	1000
Toluene with prodcut to stage 2	941		Rec. Toluene	3026
4-Fluro 3-Phenoxy Benzaldehyde	430		Aq. Effluent	1605
Sodium Cynide	222	→	Residue	89
Toluene	2174			
Sodium Bisulphite	111			
Water	1213			
Tetraytyl ammonium Bromide	2			
	5720			5720

Energy Balance:

ENERGY BALANCE IN STR-1

Assuming all reactants are initially at room temperature, $T = 25^\circ C$.

STR-1 operates at $T = 80^\circ C$

∴ Heat required to bring reactants to reaction temperature:

$\Delta T = 55^\circ C$ $\quad C_p\ (SOCl_2) \simeq 0.86\ KJ/kg \cdot K$

C_p (Baytico l p Acid) $\simeq 2.0\ KJ/kg \cdot K$

$C_p\ (HCl\ (aq)) \simeq 4.18\ KJ/kg \cdot K$

$C_p\ (SO_2) \simeq 0.62\ KJ/kg \cdot K$

$$\boxed{\dot{Q} = \dot{m} C_p \Delta T}$$

$$\dot{Q}_{BPA} = 653\ \frac{kg}{day} \times 2\ \frac{KJ}{kg \cdot K} \times 55\ K = 71830\ KJ/day$$

$$\dot{Q}_{SOCl_2} = 276\ \frac{kg}{day} \times 0.86\ \frac{KJ}{kg \cdot K} \times 55K = 13099\ KJ/day$$

$$\therefore \dot{Q}_{total\ req} = 84929\ KJ/day \simeq 85000\ KJ/day$$

$\Delta H_{rxn-1} \simeq -50\ KJ/mol$, $2.3\ kmol/day$ of Baytico l P Acid ~~Chloride~~

$$\therefore \Delta H = 50\ \frac{KJ}{mol} \times 2.3\ \frac{kmol}{day} = -115000\ KJ/day$$

This reaction is Exothermic.

$$\therefore \dot{Q}_{net} = 85000 - 115000\ KJ/day = -30000\ KJ/day$$

$$\boxed{\dot{Q}_{net} = -30000\ KJ/day}$$

ENERGY BALANCE IN STR-2

- Assuming all reactants are initially at room temperature, $T = 25°C$, STR-2 operates at $T = 60°C$

$\therefore$ Heat required to bring reactants to reaction temperature:

$\Delta T = 35°C$

$Cp\,(4F3P) = 1.5\ KJ/kg \cdot K$

$Cp\,(\text{Baytical P-Acid Chloride}) = 1.3\ KJ/kg \cdot K$

$Cp\,(NaCN) = 1.44\ KJ/kg \cdot K$

$$\boxed{\dot{Q} = \dot{m} C_p \Delta T}$$

$\dot{Q}_{4F3P} = 471 \frac{kg}{day} \times 1.5 \frac{KJ}{kg \cdot K} \times 35\,K = 24727.5\ KJ/day$

$\dot{Q}_{BPAC} = 661 \frac{kg}{day} \times 1.3 \frac{KJ}{kg \cdot K} \times 35\,K = 30003\text{9}.5\ KJ/day$

$\dot{Q}_{NaCN} = 108 \frac{kg}{day} \times 1.44 \frac{KJ}{kg \cdot K} \times 35\,K = 5443.2\ KJ/day$

$\dot{Q}_{\text{total req}} \simeq 60200\ KJ/day$

$\Delta H_{rxn-2} \simeq -75\ KJ/mol$, $2.2 \frac{kmol}{day}$ of 4F3P

$\therefore \Delta H = -75 \frac{KJ}{mol} \times 2.2 \frac{kmol}{day} = -163350\ KJ/day$

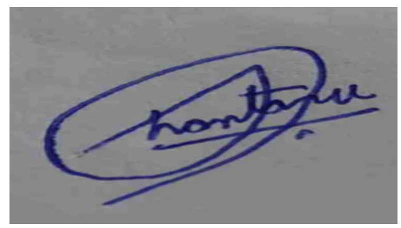
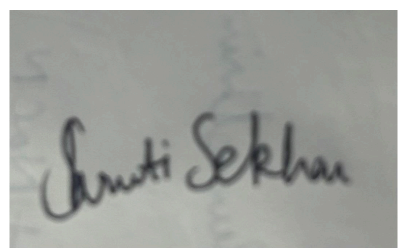
$\therefore \dot{Q}_{net} = -163350 \frac{KJ}{day} + 60200\ KJ/day$

$$\boxed{\dot{Q}_{net} = -103990\ KJ/day}$$

List of Contributions of each author:

P. Shruti Sekhar : Identified the chemical Flumethrin and the reactions involved in its production. Designed the process flow sheet and did the stoichiometric mass balance and drafted the technical patent.

Shantanu Prakash : Identified reactor types and other unit operations, estimated yield. Complete Stoichiometric Material balance , Energy balance and drafted the technical patent .

Name	Roll No	Signature
Shantanu Prakash	230952	
P Shruti Sekhar	230723	
Kumar Shubham	230587