CHE 261

Chemical Process Industries

Instructor: Prof. Raghavendra Ragipani

GROUP PROJECT PRESENTATION

TEAM: VortexChem

TEAM MEMBERS

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R&D

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MARKET ANALYSIS

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EHS

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WORK-FLOW

1 CHEMICAL PATENTING

R&D team screened chemicals on different parameters to finally come up with three chemicals

2 MARKET ANALYSIS

Marketing team worked on economic feasibility of 2 of these chemicals

3 PROCESS PATENTING

Technical team found best fit processes for the selected chemicals

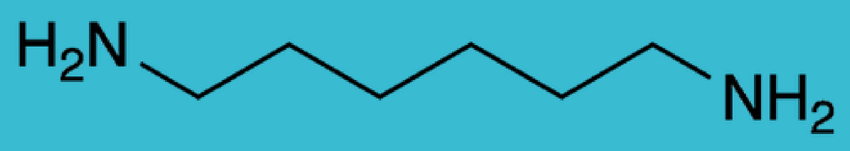
4 ENVIRONMENTAL CLEARANCE

EHS team formulated the EHS reports and applied for clearance

CHEMICALS PATENTED

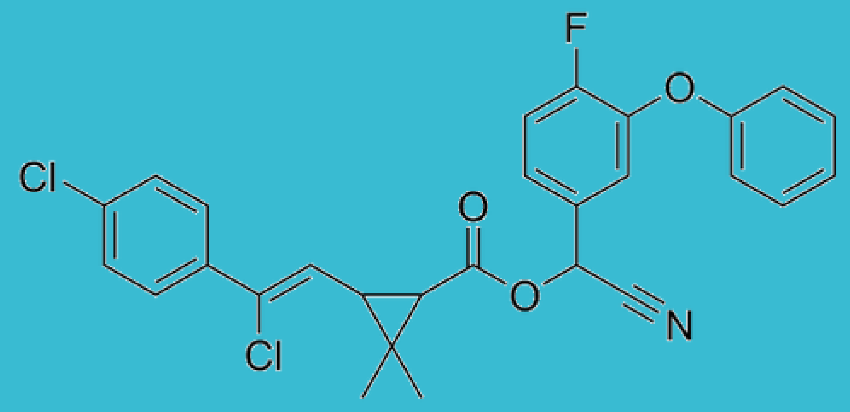
Hexamethylenediamine (HMDA)

A specialty fine chemical used mainly in nylon 6,6, coatings, and polymers



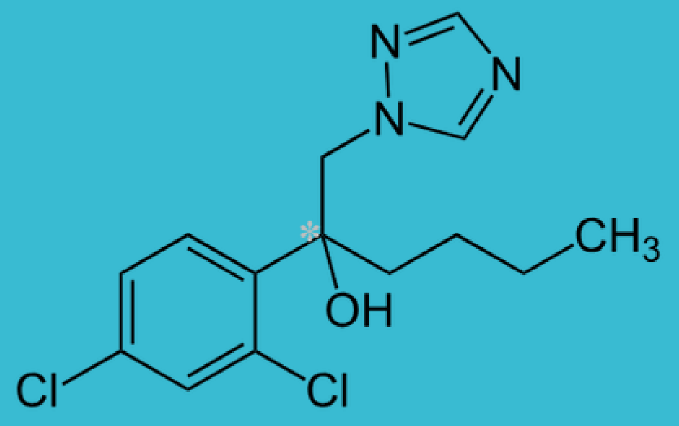
Flumethrin

Agrochemical – Synthetic pyrethroid insecticide and acaricide used to control ticks and mites on livestock



Hexaconazole

Agrochemical (Fungicide - triazole class) - Controls fungal diseases in crops like rice, wheat, etc.



CHEMICALS PATENTED

Parameters \ Chemicals	HMDA	Flumethrin	Hexaconazole
Key Raw Materials	Adiponitrile, Hydrogen, Ammonia	Bayticol P Acid, Thionyl chloride, Sodium cyanide, 4-fluoro-3-phenoxybenzaldehyde	Valeryl Chloride, MDCB, 1,2,4-Triazole, Dimethyl sulphate, KOH
Major Reaction Steps	Hydrogenation of adiponitrile	1. Acid chloride formation 2. Nucleophilic substitution with cyanide and aldehyde	1. Acylation 2. Epoxide (Oxirane) formation 3. Nucleophilic substitution with triazole
Typical Theoretical Yield (%)	~93–95%	Step 1: ~95% Step 2: ~90%	Acylation: ~95.8% Epoxidation: ~95.6% Final: ~83.3%
Conditions	High pressure, ~100–200°C	Step 1: 80–100°C (reflux, inert) Step 2: 50–70°C	Step-wise: 303K (Acylation), 333K (Oxirane & Final), low pressure (0.5 atm)

KEY INSIGHTS

We proceeded to further analyse two of our chemicals mainly due to availability of resources:

- **Flumethrin**
- **Hexaconazole**

MARKET

HEXACONAZOLE	PARAMETERS	FLUMETHRIN
₹1,425/kg	**Production Cost (per kg)**	₹417/kg
₹2,700	**Selling Price (per kg)**	₹700
₹1,275	**Gross Profit (per kg)**	₹283
~47.2%	**Profit Margin**	**~40%**
Moderate – solvents like DMF/toluene used	**Solvent Recovery Importance**	High – toluene recovery emphasized to cut costs
RM price fluctuations, import dependency, regulation	**Economic Risk Factors**	Hazardous intermediates, export decline, price volatility

KEY INSIGHTS

TECHNICAL

Material Balance has been done to calculate E-Factor

1. FLUMETHRIN

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

Waste Considered(since we are not recycling anything for now):

- HCl gas
- SO_2 gas
- Aqueous Effluent
- Residue
- Rec Toluene

E- FACTOR = 4.33

Waste Considered(since we are not recycling anything for now):

- Aqueous Effluent
- Residue
- Rec Toluene

E- FACTOR = 4.72

KEY INSIGHTS

2. HEXACONAZOLE

Step-1: Preparation of Valerophenone:

Material Balance:

Input	Kg		Output	Kg
Meta Di Chloro Benzene	1500		Valerophenone	924
Velaryl Chloride	503		Meta Di Chloro Benzene rec.	574
Aluminium Chloride	733	Step-1	Aq. Waste to ETP	1452
Water	2637		Al(OH)3	2393
			Residue	30
	5373			5373

Waste Considered:
- Aqueous waste to ETP
- Residue
- $Al(OH)_3$

E- FACTOR = 4.19

Step-2: Preparation of Oxirane:

Material Balance:

Input	Kg		Output	kg
Valerophenone	924		Oxirane	937
KOH	531		DMS Rec.	1455
DMSO4	602		K2SO4	898
DMS	1476	Step-2	EDC Rec	1182
EDC	1250		Aq. Waste to ETP	2195
Water	1884			
	6667			6667

Waste Considered:
- K_2SO_4
- Aqueous waste to ETP

E- FACTOR = 3.30

Step-3 Preparation of Hexaconazole:

Material Balance:

Input	Kg		Output	Kg
Oxirane	937		Hexaconazole	1000
DMF	3562		DMF Rec	3289
KOH	67		KOH	71
Triazole	299	Step-3	Methanol Rec	1405
Methanol	1560		Residue	440
Water	2000		Aq. Waste to ETP	2220
	8425			**8425**

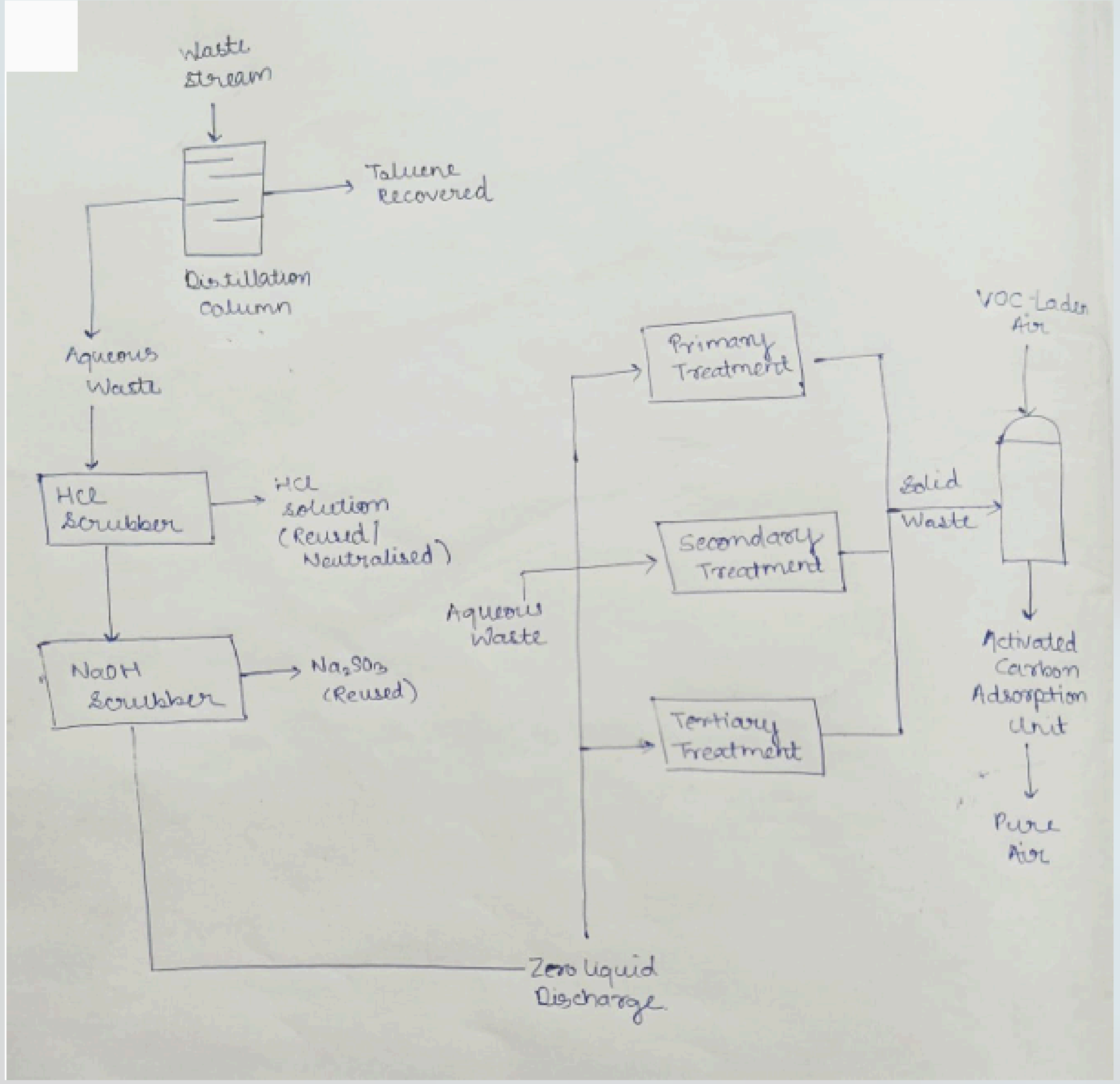
Waste Considered:
- Residue
- Aqueous waste to ETP
- KOH

E- FACTOR = 2.73

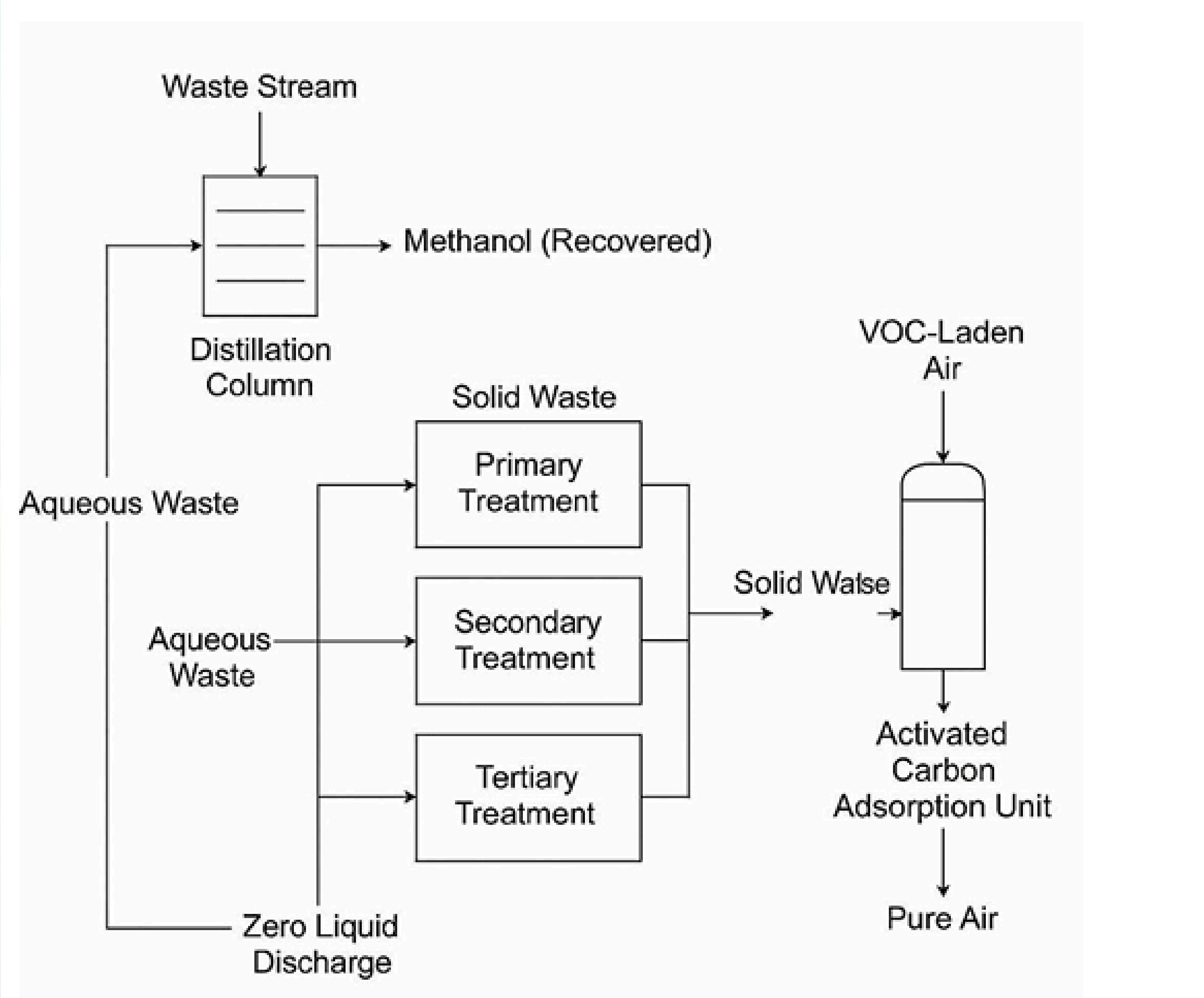
KEY INSIGHTS

EHS

1. FLUMETHRIN



2. HEXACONAZOLE



Both the chemicals are toxic if exposed without treating hence we proposed a recycling method for them

APPENDIX

VERTICAL WISE ASSESSMENT

R&D

Hexamethylenediamine (HMDA)

Key Inputs

- Adiponitrile (ADN): $NC-(CH_2)_4-CN$
- Hydrogen Gas (H_2)
- Ammonia (NH_3): Acts as both suppressor of side reactions and hydrogen solubility enhancer
- Catalysts: Raney Nickel or Raney Cobalt
- Reaction Medium: Water
- Utilities: Cooling water for thermal regulation

Reaction Pathway

1. Partial Hydrogenation – Formation of Intermediate
2. $NC-(CH_2)_4-CN + 2H_2 \rightarrow H_2N-(CH_2)_4-CN$ (6-Aminohexanenitrile)
3. Complete Hydrogenation – Final Product
4. $H_2N-(CH_2)_4-CN + 2H_2 \rightarrow H_2N-(CH_2)_6-NH_2$ (HMDA)

Yields

- Raney Ni Catalyst: Up to >90% under optimal conditions
- Raney Co Catalyst: Typically 85–87%

VERTICAL WISE ASSESSMENT

R&D

FLUMETHRIN

Synthesis Methodology:

Step 1: Preparation of Bayticol P Acid Chloride

- Reaction:
- Bayticol P Acid + Thionyl Chloride ($SOCl_2$)
- Catalyst: Dimethylformamide (DMF)
- Solvent: Toluene
- Conditions: Reflux at 80–100°C under nitrogen atmosphere
- By-products: Sulfur dioxide (SO_2) and hydrogen chloride (HCl), scrubbed with aqueous NaOH
- Isolation: Vacuum distillation
- Yield & Purity: ~95% yield, >98% purity

Step 2: Formation of Flumethrin

- Reaction:
- Bayticol P Acid Chloride + Sodium Cyanide (NaCN) + 4-fluoro-3-phenoxybenzaldehyde
- Catalyst: Tetrabutylammonium Bromide (TBAB – phase-transfer catalyst)
- Solvent: Toluene
- Conditions: 50–70°C, followed by aqueous workup, filtration, crystallization, and controlled drying
- Yield & Purity: ~90% yield, 90–100% purity

VERTICAL WISE ASSESSMENT

R&D

FLUMETHRIN

Key Insights:

- Optimized temperature control and catalyst concentration significantly improve yield and purity.
- Solvent recovery (toluene) reduces environmental load and operational costs.
- Efficient scrubbing of acidic gases ensures safety and compliance.
- High product quality is achieved through vacuum distillation, aqueous extraction, and recrystallization.

VERTICAL WISE ASSESSMENT

R&D

HEXACONAZOLE

Synthesis Methodology:

Step 1: Formation of Valerophenone (Acylation)

- Reaction:
- 2,4-Dichlorobenzyl Chloride + Valeryl Chloride
- Catalyst: Aluminium Chloride ($AlCl_3$)
- Conditions: 303 K, atmospheric pressure
- Yield: ~95.8%
- Purification: Solvent removal via rotary evaporation, followed by distillation

Step 2: Oxirane Formation (Epoxidation)

- Reagents: Dimethyl Sulfate + Dimethyl Sulfide
- Alternative: mCPBA (meta-chloroperoxybenzoic acid) for greener synthesis
- Conditions: 333 K, 0.5 atm
- Workup: Neutralization using KOH
- Yield: ~95.6%

VERTICAL WISE ASSESSMENT

R&D

HEXACONAZOLE

Step 3: Hexaconazole Formation (Ring Opening)

- Reaction:
- Oxirane intermediate + 1,2,4-Triazole
- Solvent: Dimethylformamide (DMF)
- Catalyst/Base: TBAB + KOH
- Conditions: 333 K, 0.5 atm
- Purification: Crystallization using toluene/chloroform → Filtration → Drying
- Yield: ~83.3%

Key Insights:

- Controlled temperature and phase-transfer catalysis (TBAB) are critical for yield efficiency.
- Solvent recycling and neutralization protocols make the process more sustainable.
- mCPBA offers a greener epoxidation route compared to traditional reagents.
- Multi-stage purification ensures a high-quality end product suitable for agrochemical applications.

VERTICAL WISE ASSESSMENT

MARKET ANALYSIS

FLUMETHRIN

Chemicals Chosen (Reason for Selection)

- It is used on animals to kill ticks, fleas, and lice.
- Beekeepers use it to protect bees from mites.
- It helps in public health by killing mosquitoes and flies.
- It is used in poultry and dairy farms to keep animals healthy.

Approach for Market Analysis

- Looked at where and how it is used.
- Compared it with other similar chemicals.
- Checked import/export data.
- Studied how it is made and what is needed.
- Found costs of raw materials.
- Checked selling price.
- Calculated profit after losses in production.

VERTICAL WISE ASSESSMENT

MARKET ANALYSIS

FLUMETHRIN

Key Parameters Considered

- India's import and export numbers.
- Prices of raw materials.
- Cost to make Flumethrin.
- Market selling price.

Learnings and Risks

Learnings and Risks
What was learned:
·– Studying chemistry, price, and demand gives a clear view.
·– Reusing solvents saves money.
·– Good production yield is important for profit.
Risks:
·– Some raw materials are dangerous and need care.
·– Export numbers dropped this year.
·– Some countries may have strict rules.
·– Prices can change suddenly.

VERTICAL WISE ASSESSMENT

MARKET ANALYSIS

HEXACONAZOLE

Chemicals Chosen (Reason for Selection)

- Broad-spectrum fungicidal properties (effective against sheath blight, rust, powdery mildew, etc.)
- Systemic action (long-lasting protection with low dosage)
- Plant growth-promoting effects (unlike Tebuconazole or Azoxystrobin)
- Economic feasibility (high profit margins ~47.2% in production)
- Market demand (rising imports in India, ~80–130 MT projected for 2024)

Approach for Market Analysis

- Use Case Identification: Agricultural, horticultural, and post-harvest applications
- Competitor Benchmarking: Compared with Tebuconazole, Azoxystrobin (efficacy, cost, resistance management)
- Trade Data Review: Import/export trends (China as top supplier; exports to Vietnam, China)
- Economic Feasibility: Raw material costs, production expenses, profit margins

VERTICAL WISE ASSESSMENT

MARKET ANALYSIS

HEXACONAZOLE

Key Parameters Considered

- Technical Performance: Systemic action, dosage efficiency, residual effect
- Market Dynamics: Import reliance (70% from China), export potential (USD 20–50M/year)
- Cost Structure: Raw material pricing (e.g., MDCB at ₹500–600/kg), solvent/catalyst costs
- Regulatory and Resistance Risks: Lower resistance risk compared to Carbendazim

Learnings and Risks

Learnings

- Dual role (fungicide + growth promoter) increases marketability
- Local production can reduce import dependency and meet export demand

Risks

- Supply chain dependency on Chinese raw materials (e.g., Valeryl Chloride)
- Regulatory uncertainties on triazole fungicides
- Risk of fungal resistance due to overuse

VERTICAL WISE ASSESSMENT

TECHNICAL

Process Flowsheet : From the selected reactions, we manually constructed a complete process flowsheet from scratch. This involved mapping out all necessary unit operations including reactors, separation units, and scrubbing systems to ensure the synthesis of the final product from given raw materials. Special attention was paid to the handling of key intermediates and by-products, ensuring the process design is both feasible and industrially relevant.

Mass Balance : We also carried out a complete stoichiometric mass balance from scratch for each reaction involved in the multi-step synthesis. This included manual adjustments based on reaction efficiencies and yields at each stage. The final stoichiometric mass balance data were then compared to relevant industrial data currently in use, and any discrepancies observed were analyzed with probable reasons discussed in detail.

Energy Calculations : This included estimating the sensible heat required to raise the temperature of reactants and approximating the heat released from all exothermic reactions. We also explored the possible utilization of this excess energy within the process to improve overall energy efficiency.

VERTICAL WISE ASSESSMENT

EHS

1. Waste Quantification

Based on process flow diagrams and mass balances provided by the **Technical and R&D teams**, we calculated the **waste generation** during formation of Hexaconazole and Flumethrin. This allowed us to estimate total waste intensity and design appropriate treatment strategies.

2. Regulatory Benchmarking

We researched **exposure limits and regulatory guidelines** for all major waste chemicals using OSHA, ACGIH, and NIOSH references.

These values helped us align the waste handling procedures with **permissible exposure and discharge limits**.

3. Waste Treatment Design

We collaborated on preparing the **block diagram for waste treatment**, ensuring that all streams met ZLD criteria. We used techniques and methods like distillation, MEE (Multiple Effect Evaporator), crystalliser to treat aqueous waste. We also ensured solid waste segregation and treatment based on hazard classification. We used VOC (Volatile Organic Compounds) Control for vapor waste treatment.

This integrated strategy allowed us to achieve a **zero discharge** and environmentally safe process.

Thank You