

SynTech

CHE 261 : Virtual Company

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In This Presentation...

- **We will cover the production, market analysis, and environmental impact of three chemicals:**
 - ▶ **Methylene Diphenyl Diisocyanate (MDI)**
 - ▶ **PolyVinyl Chloride (PVC)**
 - ▶ **2,5-Furandicarboxylic Acid (FDCA)**

Methylene Diphenyl Diisocyanate

Overview

- **Chemical : MDI**
- **Chemical Formula : C₁₅H₁₀N₂O₂**
- **Uses :**
 - **Used in polyurethane foam production.**
 - **Found in adhesives, coatings, elastomers, and sealants.**

Production

Traditional Phosgenation Method

- Aniline and formaldehyde react to form diphenylmethane diamine (MDA) under acidic conditions. The reaction typically occurs at 60-110°C and 1-5 bar pressure, producing a mixture of MDA isomers and oligomers.
- MDA is then reacted with phosgene (COCl_2) in an inert solvent like dichloromethane or toluene. The phosgenation reaction takes place at temperatures between 50-250°C and pressures up to 50 bar. This step converts the amine groups ($-\text{NH}_2$) of MDA to isocyanate groups ($-\text{NCO}$), forming MDI.
- Hydrogen chloride (HCl) is produced as a byproduct and is typically recycled.
- The crude MDI mixture undergoes rectification (purification) through distillation and side rectification to separate different isomers. The process operates under extreme vacuum (2-10 mBar) to minimize operating temperature and preserve product quality.
- The final product typically contains at least 98.5% by weight of 4,4'-MDI, the most desirable isomer.

Phosgene Free Method

- This method uses MDA, 3-methyl-1-butanol (3-MB), and urea as primary reactants.
- In the first step, MDA reacts with 3-MB and urea at 428 K and 100 kPa to form a carbamate intermediate (3-MBE). This reaction achieves 100% conversion of MDA with 95% selectivity to 3-MBE.
- Ammonia is produced as a byproduct and is separated along with excess 3-MB.
- The second step involves thermal decomposition of 3-MBE at 493 K and 100 kPa to form MDI. This decomposition also produces 3-MB (which is recycled) and 2,4-di-tert-butylphenol (DTB) as byproducts.
- The process requires efficient separation and recycling systems for unreacted materials and solvents.
- Overall yield is approximately 90% MDI after optimization and recycling.
- This method eliminates the use of highly toxic phosgene, making it a safer and more environmentally friendly alternative. However, it requires careful management of recycle streams and byproducts to maintain economic viability.

PolyVinyl Chloride

Overview

- **Chemical : PVC**
- **Chemical Formula : $(C_2H_3Cl)_n$**
- **Uses :**
 - **Plumbing pipes and fittings**
 - **Electrical wire insulation**
 - **Construction materials (windows, doors, roofing)**
 - **Medical devices**
 - **Packaging**

Profitability

Market Analysis

- **India imports \$2.71 billion worth of PVC annually.**
- **22% import growth over two decades.**
- **Global market valued at \$68.96 billion in 2022.**
- **Global market expected to grow to \$95.88 billion by 2030.**
- **Expected CAGR of 4.2% from 2023 to 2030.**
- **Asia Pacific dominates with 56.19% market share.**
- **For production via suspension method, we get 40.59% profit margin.**
- **However, the profitability of PVC production in India depends on global raw material prices, import duties, and domestic production expansion.**

Production

VCM Production

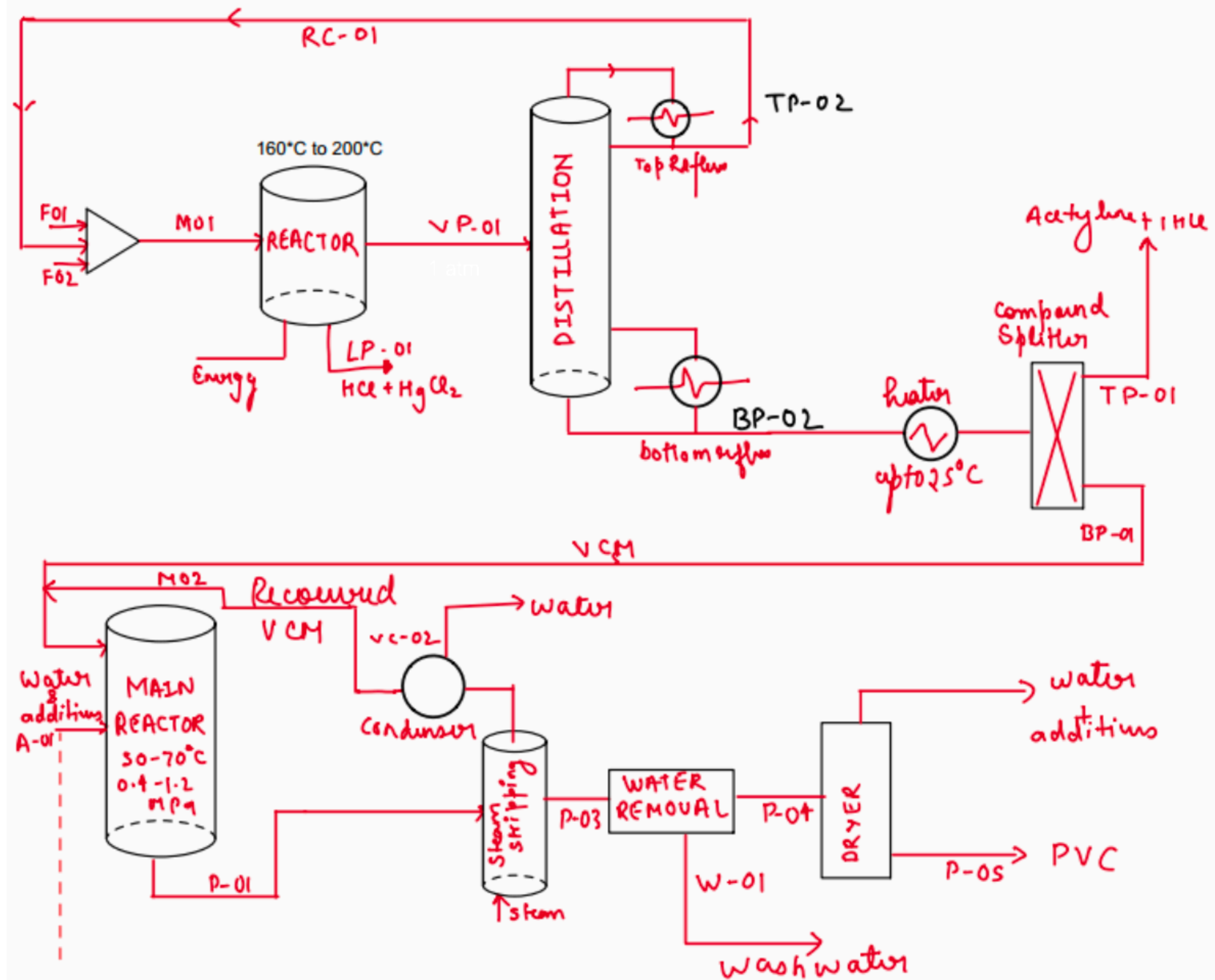
- VCM is the primary raw material for PVC production and is synthesized via two methods:
- **Thermal Cracking of Ethylene Dichloride (EDC):**
 - Ethylene reacts with chlorine to form EDC.
 - EDC is then thermally cracked at 450–550°C and 15–30 atm to produce VCM and hydrogen chloride.
 - **Oxychlorination Process:** Recycles HCl by reacting with oxygen and ethylene over a copper-based catalyst at 200–250°C to form more EDC.
 - Thermal cracking method achieves 85-95% conversion efficiency.
- **Hydrochlorination of Acetylene:** acetylene reacts with hydrogen chloride at 150–200°C with a mercury-based catalyst to form VCM.
- Thermal cracking of EDC is preferred over acetylene hydrochlorination due to lower raw material cost and environmental concerns with mercury-based catalysts.
- **VCM Purification:** After synthesis, VCM is purified via distillation to remove impurities. Side products can be used for chlorinated solvents or catalytically oxidized.
- **VCM Storage & Transport :** Stored as a pressurized liquid to prevent polymerization. Strict safety measures are required due to its carcinogenic and flammable nature.

Suspension polymerization

- **VCM is polymerized in an aqueous medium, forming PVC particles suspended in water.**
- **We use initiators (peroxides, azo compounds) for free radical polymerization, suspending agents (polyvinyl alcohol, gelatin)** to stabilize droplets and water as the continuous phase.**
- **Reactor is sealed and purged with nitrogen or vacuum to remove oxygen. VCM is introduced, and the reactor is heated to 50-70°C at 0.4 - 1.2 MPa for polymerization.**
- **Free radicals react with VCM to start polymer chains. Chain growth continues with more VCM addition. Two polymer chains combine, ending the reaction.**
- **After reaching 85-97% conversion, unreacted VCM is removed by vacuum stripping and recycled.**
- **PVC slurry is washed to remove residual chemicals. The polymer is dewatered via centrifugation or filtration. Hot air drying (fluid bed/rotary dryer) removes moisture.**
- **Sieving and filtration ensure uniform particle size.**
- **PVC is processed into pellets, sheets, or pipes depending on the application.**
- **85-97% VCM conversion to PVC.**
- **Most widely used PVC production method due to cost-effectiveness and scalability.**

Emulsion polymerization

- **Emulsion polymerization produces fine PVC particles (50-300 nm) for coatings, adhesives, and specialty applications.**
- **We use surfactants (sodium lauryl sulfate, alkyl sulfonates) to stabilize emulsion, water-soluble initiators (persulfates, redox systems) for free radical polymerization and protective colloids (polyvinyl alcohol) for additional stabilization.**
- **VCM is dispersed in water using surfactants under agitation to create monomer droplets (50-200 nm).**
- **Persulfates ($K_2S_2O_8$) or redox systems generate free radicals, starting polymerization.**
- **Radical attack on VCM initiates polymer chains. Growth continues inside micelles or dispersed monomer droplets. Polymer chains stabilize within latex-like dispersion.**
- **Radical termination leads to stable PVC latex. Latex contains 40-60% solid PVC.**
- **Electrolytes (salts) or acids coagulate latex. Filtered, washed, and dried to recover solid PVC.**
- **We do fine grinding for uniform particle size. pH neutralization of PVC to remove acid traces.**
- **Residual VCM stripping to reduce toxicity (<1 ppm after stripping).**
- **80-95% VCM conversion per batch.**



Sustainability

Environmental Impact

- **Waste Generation**

- **Unreacted Acetylene:** 13 kg/day, flammable and asphyxiant gas.
- **Hydrogen Chloride (HCl) Gas:** 18.2 kg/day, highly corrosive and hazardous to the respiratory system.
- **Benzyl Alcohol (Additive Waste):** 6.633 kg/day, exposure can cause dizziness, nausea, and respiratory issues.
- **Wastewater:** 2222.2 kg/day, containing water from various process units.
- **Mercuric Chloride (HgCl₂) Catalyst Residue & Unreacted Vinyl Chloride Monomer (VCM):** Present in small quantities, both highly toxic and carcinogenic.

- **Regulatory Compliance**

- **Acetylene Regulations:** TWA (8-hour) = 2500 ppm, requires ventilation and ignition control to prevent fire hazards.
- **HCl Gas Limits:** Ceiling limit = 5 ppm, requires neutralization using sodium bicarbonate and PPE for handling.
- **Mercuric Chloride Regulations:** 0.01 mg/m³ exposure limit; requires hazardous waste handling due to toxicity and bioaccumulation risks.
- **Vinyl Chloride Monomer (VCM) Limits:** Carcinogenic, TWA = 1 ppm, Ceiling = 5 ppm, strictly controlled under occupational health regulations.
- **Benzyl Alcohol Limits:** TWA = 10 ppm, STEL = 20 ppm, requires **PPE and exposure minimization.

- **Safety Concerns**

- **Acetylene Hazards:** Can cause asphyxiation and dizziness at high concentrations.
- **HCl Exposure Risks:** Causes severe respiratory tract irritation; prolonged exposure may lead to pulmonary edema.
- **Mercuric Chloride Toxicity:** Severely toxic, potential carcinogen, can lead to kidney damage and respiratory failure.
- **VCM Dangers:** Carcinogenic and flammable, prolonged exposure linked to liver and kidney damage.

Treatment Plan

- **Wastewater Treatment:** Removal of neutralization, and closed-loop water recycling.
- **Vent Gas Treatment:** Scrubbers for HCl neutralization, activated carbon for VCM adsorption, and proper ventilation to remove acetylene safely. Fine PVC dust emissions (0.5-2 kg per ton) controlled by bag filters.
- **HgCl₂ and VCM Separation:** Chemical precipitation and filtration for HgCl₂ recovery, while VCM is stripped and recycled.
- **Unreacted VCM Stripping:** Vacuum stripping technology ensures that VCM levels in the final PVC product are minimized (<1 ppm).
- **Zero Liquid Discharge (ZLD) Compliance:** Surfactant residues and high Chemical Oxygen Demand (COD) in wastewater. Process water is filtered, neutralized, and reused, ensuring no untreated wastewater discharge into the environment.

2,5-Furandicarboxylic Acid

Overview

- **Chemical : FDCA**
- **Chemical Formula : $\text{C}_6\text{H}_4\text{O}_5$**
- **Uses :**
 - **bio-based alternative to Terephthalic Acid in PET production**
 - **Key ingredient in polyesters, antibacterial agents, and fire foams**
 - **Used in artificial veins and kidney stone treatments.**
 - **Chelating agent for metal ions**

Profitability

Market Analysis

- **India imports large amounts of TPA, FDCA can be a potential replacement.**
- **Growth driven by increasing demand for sustainable plastics.**
- **Global market projected to reach \$67.96 billion by 2032**
- **A CAGR of 34.20% expected**
- **Advantageous over petrochemical alternatives as raw materials are renewable, it has a lower carbon footprint, and the polymers produced have superior quality**
- **Economic Feasibility:**
 - **Production from fructose: 52.9% profit margin**
 - **Production from biomass: 55.8% profit margin**

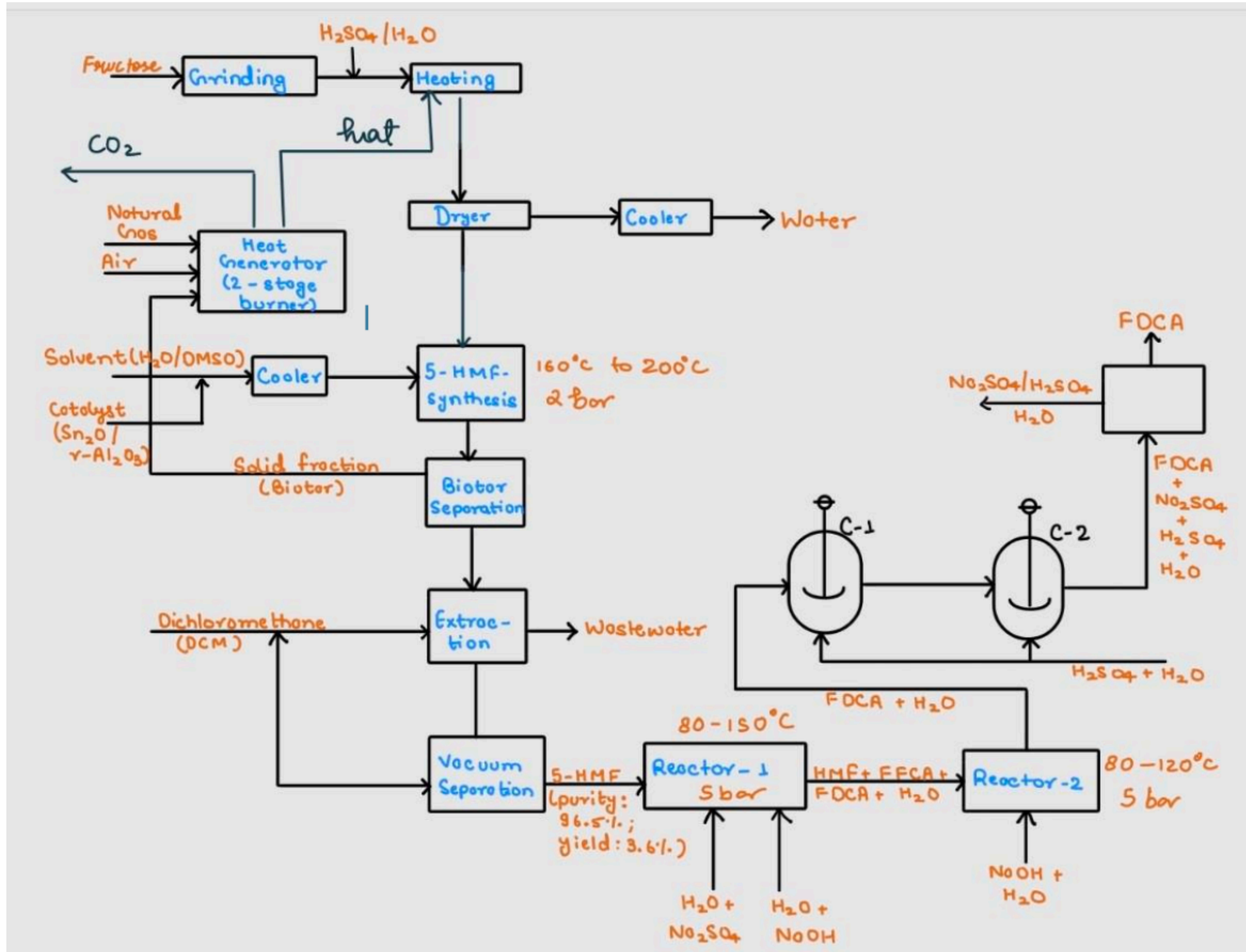
Production

Acid-catalyzed dehydration of fructose to HMF, then oxidation to FDCA

- Fructose undergoes acid-catalyzed dehydration in DMSO-H₂O with solid catalysts (Sn₂O/γ-Al₂O₃).
- The reaction produces 5-hydroxymethylfurfural (HMF) as an intermediate, which is extracted using dichloromethane (DCM).
- HMF is then oxidized to 2,5-furandicarboxylic acid (FDCA) through sequential oxidation using noble metal catalysts (e.g., AuPd, Pt, Pd).
- The oxidation process involves intermediates such as 5-hydroxymethyl-2-furancarboxylic acid (HMFCA) and 5-formyl-2-furancarboxylic acid (FFCA).
- Reaction conditions typically involve temperatures around 70-90°C for the initial oxidation steps, increasing to 110-140°C for the final conversion to FDCA.
- The overall yield of FDCA can reach up to 90% under optimized conditions.
- This process is considered more environmentally friendly compared to traditional petrochemical-based methods, as it uses renewable biomass sources and produces fewer harmful byproducts.

Biomass conversion via Furfural oxidation and carboxylation

- **Biomass (e.g., agricultural waste) is converted to furfural using SnCl_4 catalysis in a biphasic system.**
- **Furfural undergoes oxidation with a gold-based heterogeneous catalyst supported on hydrotalcite in water to produce furoic acid.**
- **The oxidation reaction achieves full conversion of furfural with high selectivity (95%) towards furoic acid within 120 minutes under optimal conditions.**
- **Furoic acid then undergoes carboxylation using carbon dioxide (CO_2) in the presence of molten cesium and potassium carbonate salts.**
- **The carboxylation reaction occurs at elevated temperatures (260-290°C) to produce FDCA.**
- **The overall yield from furfural to FDCA reaches approximately 74%, with the carboxylation step achieving about 78% yield.**
- **This method is considered more environmentally friendly as it uses non-edible biomass, water as a solvent, and incorporates CO_2 utilization. The process operates under milder reaction conditions without hazardous chemicals, aligning closely with green chemistry principles.**



Sustainability

Environmental Impact

- **Waste Generation:** The FDCA production process generates three major waste streams:
 - **Wastewater :** 369,914.25 kg/day, containing volatile organic solvents (DMSO, DCM).
 - **Acid-Water :** 310 kg/day, containing sulfuric acid (H_2SO_4) and sulfate salts (Na_2SO_4).
 - **CO₂ Emissions :** 208,051.58 kg/day.
- **Regulatory Compliance**
 - **Wastewater** must be treated to prevent groundwater contamination.
 - **Acid water** requires neutralisation due to its corrosive nature.
 - **CO₂ emissions** contribute to climate change and need mitigation strategies.
- **Safety Concerns**
 - **DMSO & DCM :** Can cause skin absorption and toxicity; regulated exposure limits exist.
 - **Sulfuric Acid :** Highly corrosive, causing potential lung damage upon prolonged exposure.
 - **CO₂ :** High concentrations can cause respiratory issues and oxygen displacement.

Treatment Plan

- **Zero Liquid Discharge (ZLD) approach is mandated.**
- **Wastewater Treatment involves solvent separation and filtration.**
- **Acid-Water Treatment Requires neutralization using a base before filtration.**
- **Volatile Organic Compounds (VOCs) Control**
- **Includes DCM, which can cause liver toxicity and contribute to air pollution.**
- **Exposure limits set at 25 ppm (OSHA PEL) with a short-term exposure limit of 125 ppm.**

Thank You