GROUP-12

STYRENE PRODUCTION

CHE251

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STYRENE PRODUCTION

Presented By : Group-12

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CONTRIBUTING MEMBERS

1. Bipin Kumar
2. Karan Keer
3. Harshit Jaiswal
4. Priyanka
5. Rutul Bhanushali
6. Pragati Patel
7. Prabhakar Raj
8. Adarsh Raj

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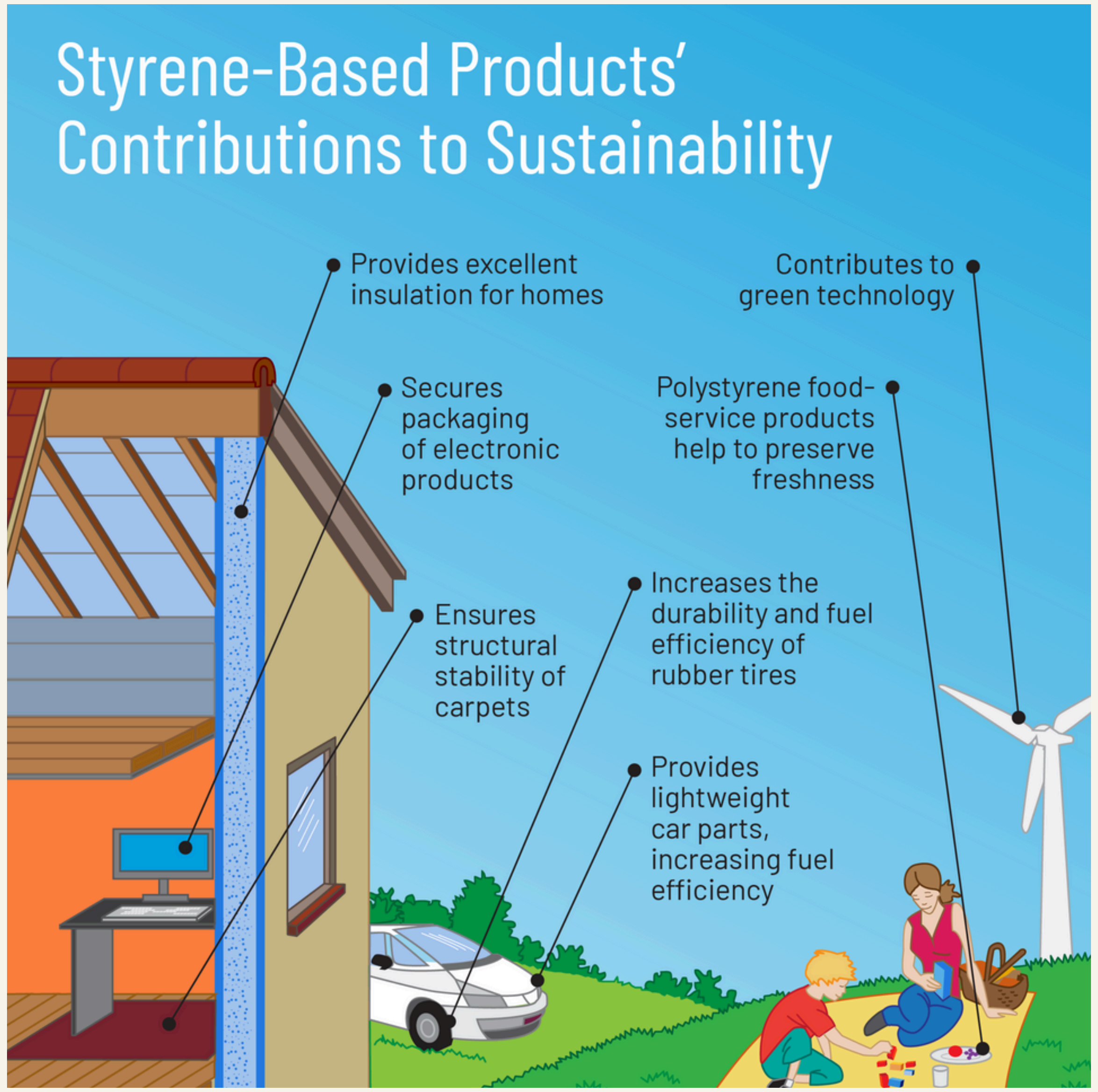
IMPORTANCE OF STYRENE



<u>Styrene</u> is a vital industrial chemical used in the production of:

- Polystyrene (used in packaging, insulation, and disposable products)
- Synthetic Rubber (used in tires, footwear, and adhesives)
- ABS Plastics (widely used in automotive, electronics, and consumer goods)

The global demand for styrene continues to grow due to its versatility in various applications, making its production economically significant.

INTRODUCTION

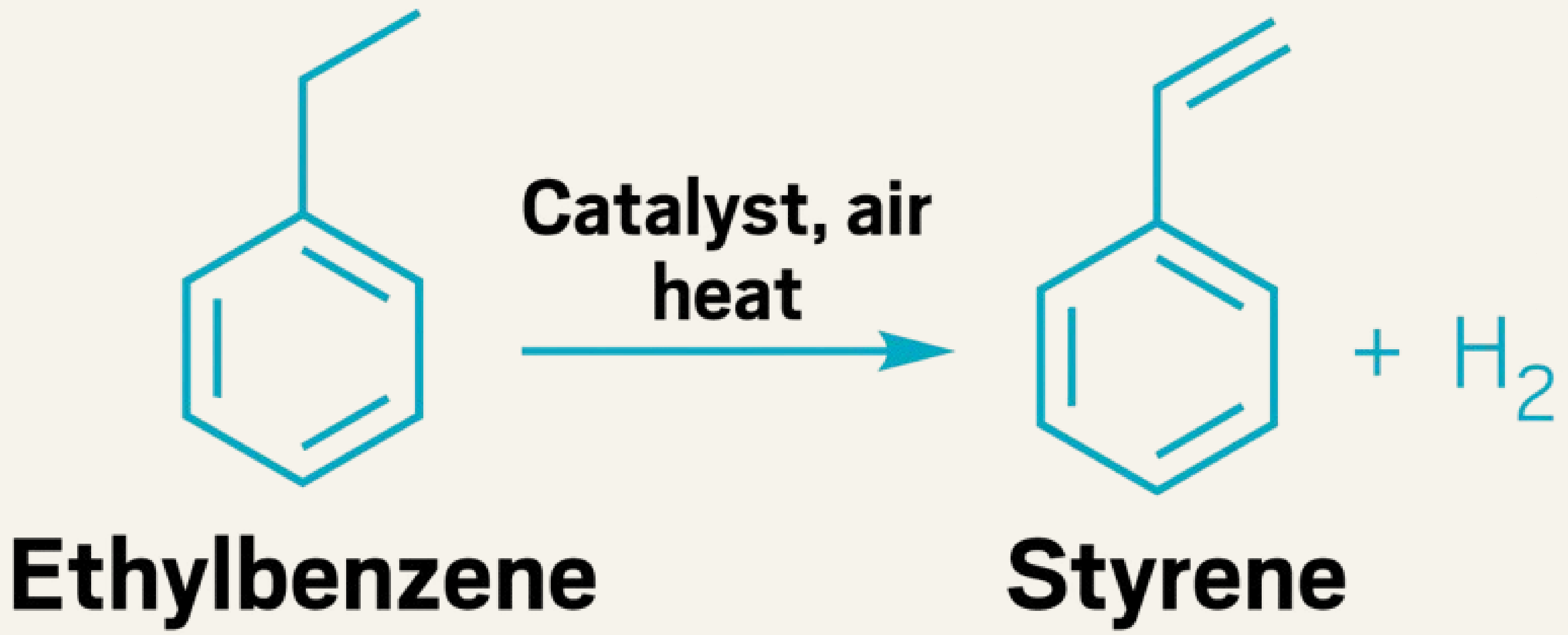
The goal of this project is to simulate the styrene production process from ethylbenzene at a mini-plant scale. The simulation will focus on optimizing reaction conditions, reactor design, and separation techniques. This will provide a foundation for understanding the industrial-scale production of styrene.

OVERVIEW

- Process Overview
- Process Flow Diagram
- Catalytic Dehydrogenation
- Mass Balance Overview
- Energy Balance Overview
- Process Optimizatiom
- Environmental Impact Analysis
- Conclusion
- Future Work

PROCESS OVERVIEW

Styrene($C_6H_5CH=CH_2$) is produced from de-hydrogenation of Ethylbenzene ($C_6H_5CH_2CH_3$). The dehydrogenation of ethylbenzene is a catalytic process that involves the removal of hydrogen atoms from ethylbenzene molecules to form styrene. This reaction is typically carried out in the vapor phase at high temperatures (around 600°C) and low pressures.



ASPEN FLOWSHEET

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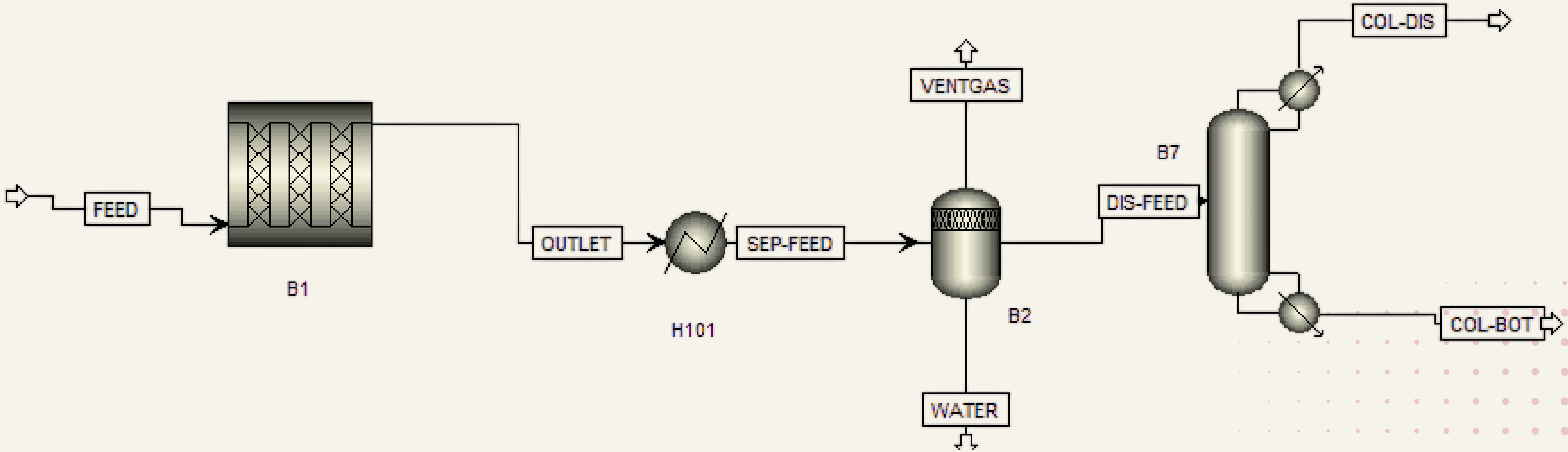
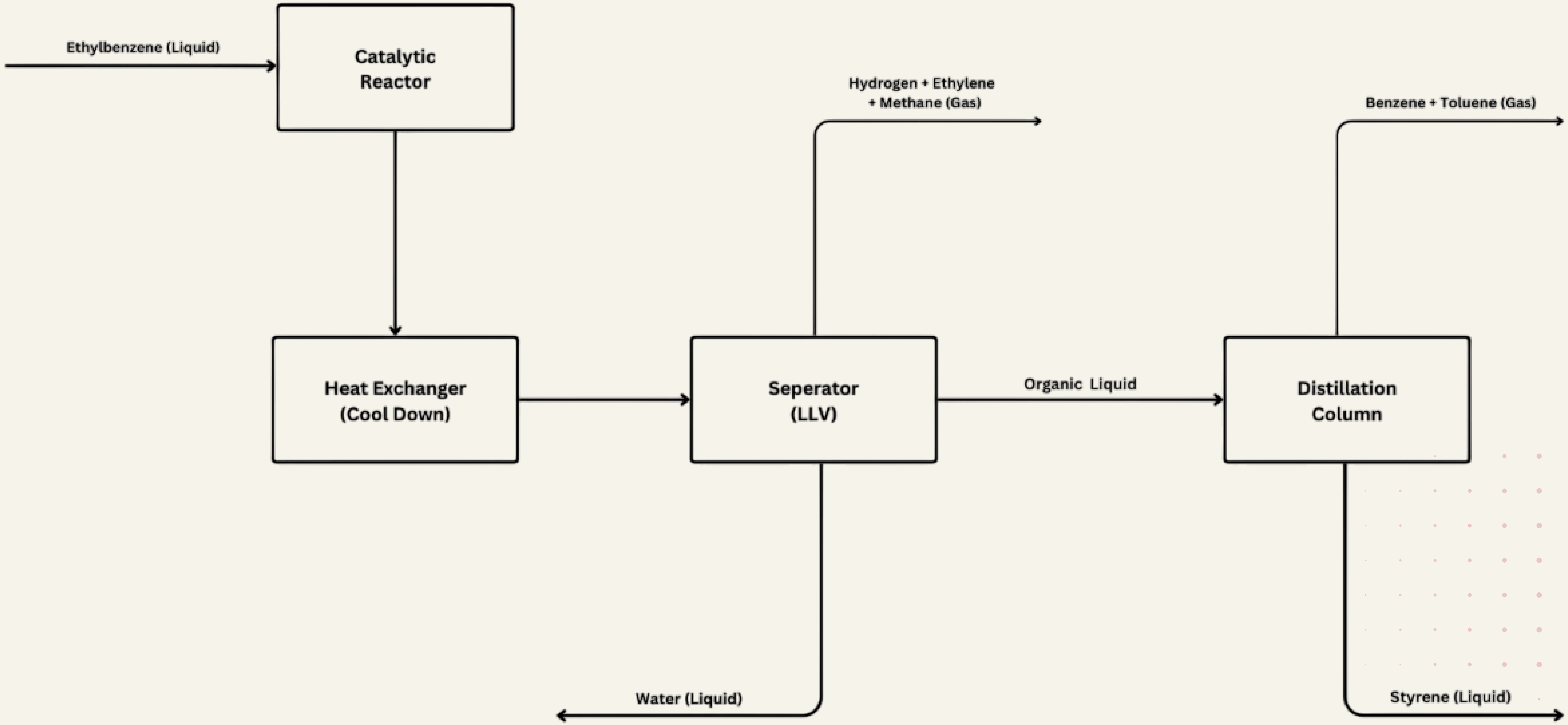
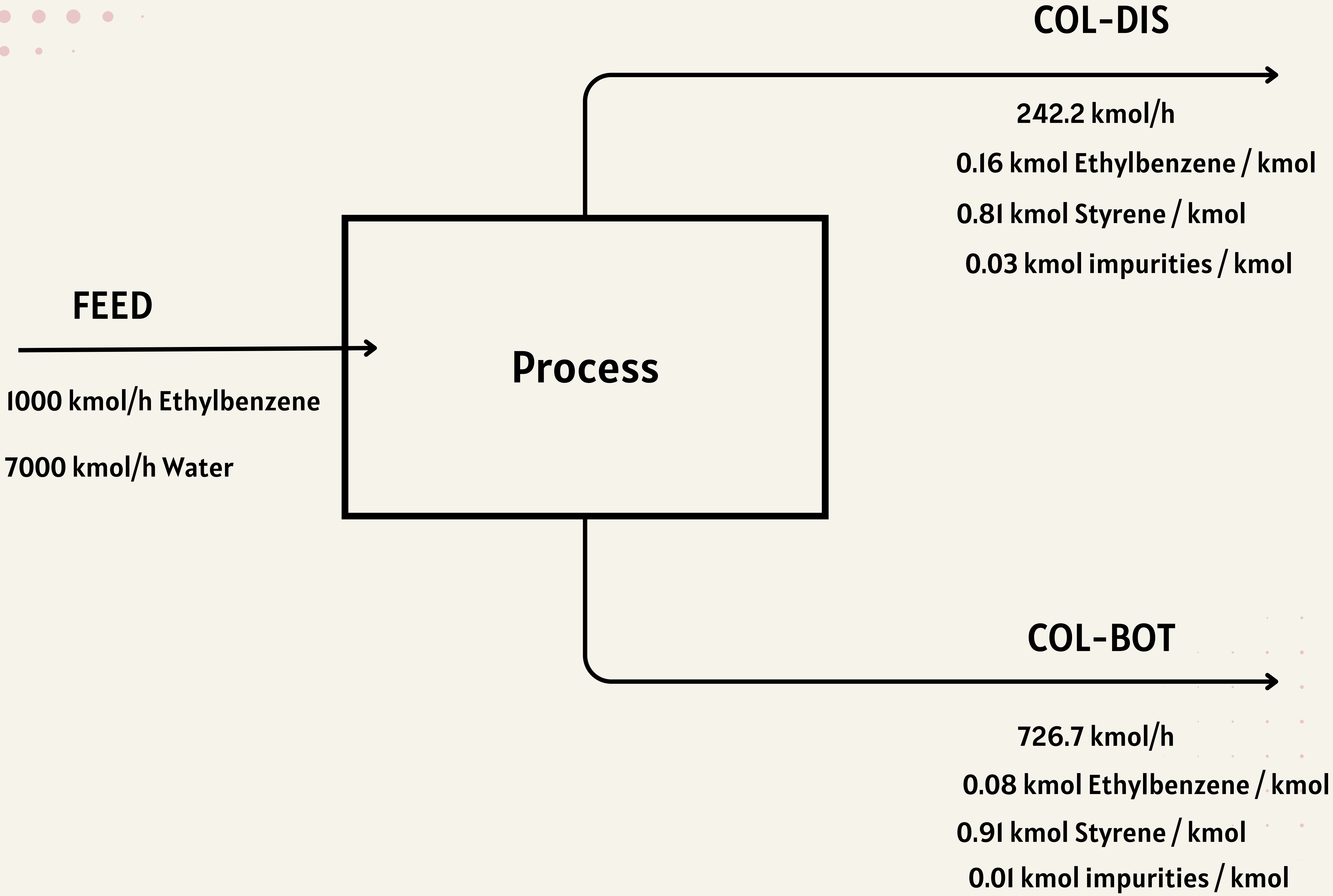


SIMPLIFIED FLOWSHEET



SIMPLIFIED FLOWSHEET



PROCESS FLOW DIAGRAM

Feed Preheating

The ethylbenzene feed is preheated to temperatures between 500°C and 600°C. This is necessary to ensure that the feed reaches the high temperatures required for the catalytic dehydrogenation reaction to occur efficiently in the next step.

Catalytic Dehydrogenation

The preheated ethylbenzene enters a fixed-bed reactor at 1 bar pressure. Inside the reactor, ethylbenzene undergoes an endothermic catalytic dehydrogenation reaction at temperatures between 600°C and 620°C, producing styrene, hydrogen, and side products like benzene, ethylene, toluene, and methane.

Heat Exchange

After leaving the reactor, the high-temperature outlet stream is cooled down to 50°C using a heat exchanger. This cooling is essential to bring the temperature down for the next separation step and to ensure that most of the organic matter and water are in their liquid phase.

Liquid-Liquid Separation

The cooled stream is then fed into the Liquid-Liquid-Volume (LLV) Separator at 50°C and 1 bar. Here, the organic and aqueous phases are separated due to their immiscibility, with the organic phase containing styrene and other hydrocarbons, and the aqueous phase primarily water.

Distillation

The organic phase from the LLV separator is sent to a distillation column. In the column, styrene (the heavy key) is separated from ethylbenzene and other light components, ensuring a high purity of the styrene product. The column is optimized with a reflux ratio of 11 and 52 stages for maximum separation efficiency.

Main Reaction

Catalytic Dehydrogenation of Ethylbenzene to Styrene

$C6H5CH2CH3 \rightleftharpoons C6H5CH{=}CH2 + H2$

Competing Reactions:

Competing thermal reactions degrade Ethylbenzene to Benzene and Ethylene.
Also , it reacts with Hydrogen to produce Toluene and Methane gas.

$C6H5CH2CH3 \rightleftharpoons C6H6 + C2H4$

$C6H5CH2CH3 + H2 \rightleftharpoons C6H5CH3 + CH4$

These are the side reactions which occur during the Production of Styrene.

MASS BALANCE OVERVIEW

Mass Conservation Principle: In any chemical process, mass is conserved. This means that the mass of the feed entering a process must equal the mass of all outputs, including desired products, by-products, and any waste streams.

Importance in Styrene Production:

- Process Control: Mass balance allows for precise control of feed and product flows, ensuring efficient conversion of ethylbenzene to styrene.
- Optimization: By tracking mass through each stage, we can minimize losses, adjust feed rates, and improve the yield of styrene while reducing unwanted by-products.
- Verification of System Integrity: Mass balance calculations confirm that all material entering each unit is accounted for, indicating stable operation without leaks or unexpected reactions.

Application in Process Simulation:

- In process simulation tools (like ASPEN), mass balance data helps model real-life operations, allowing adjustments to maximize efficiency before implementing changes in a physical plant.

ENERGY BALANCE OVERVIEW

Energy Conservation Principle: In any chemical process, energy is conserved. The energy entering a system (as heat, work, and enthalpy) must equal the energy exiting, accounting for energy changes within the process unit.

Importance in Styrene Production:

- **Endothermic Reactions:** The dehydrogenation of ethylbenzene to styrene is highly endothermic, requiring a continuous energy supply to sustain reaction temperatures.
- **Optimal Operating Conditions:** Energy balance calculations ensure that the correct amount of heat is supplied, maintaining reactor temperature without causing side reactions or thermal degradation of styrene.
- **Heat Recovery and Efficiency:** By understanding energy flow through each unit, excess heat from one stage can be reused in another, improving overall energy efficiency and reducing costs.

Application in Process Simulation:

- Energy balance data, when input into simulation tools, models realistic thermal requirements and enables optimization of energy usage, reducing operational costs and environmental impact.

Property Method for Simulation

- Goal: **Identify the best thermodynamic model for the process, given the range of pressures (0.4–1.4 bar) and high temperatures (above 600°C).**
- Initial Model: **The Peng-Robinson method is suitable for non-polar compounds but is less effective for complex systems that include both polar (water) and non-polar components.**
- Final Model Selection: **The NRTL (Non-Random Two-Liquid) model is chosen for the LLV separator as it better accounts for interactions between polar and nonpolar compounds, improving phase separation accuracy.**

PROCESS OPTIMIZATION

Optimum Operating Conditions for Distillation Column

Optimum Operating Conditions for LLV Seperator

Catalyst Selection for Dehydrogenation of Ethylbenzene

OPTIMUM OPERATING CONDITIONS FOR LLV SEPARATOR

- **Goal:** Achieve efficient separation of the organic and aqueous phases to maximize styrene yield and minimize losses.
- **Temperature Selection:** The optimum temperature is identified as 50°C. While the mole fraction of styrene in the organic phase increases with temperature, it peaks and declines sharply beyond 50°C due to vaporization, which reduces separation efficiency.
- **Water Phase Analysis:** The mole fraction of water and styrene in the water-dominant stream remains relatively stable compared to the organic stream, supporting 50°C as the optimal temperature for separation.

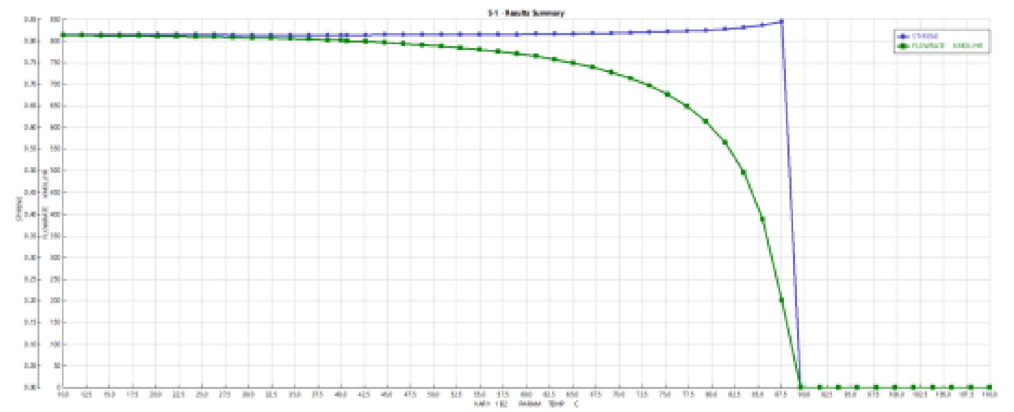


Fig-4 Mole fraction and Flowrate of Styrene in Distillation Feed

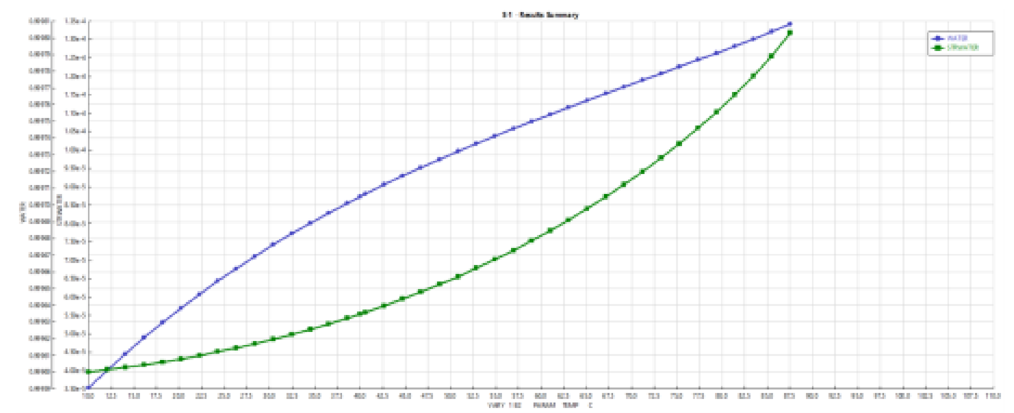


Fig-5 Mole fraction versus Temperature in Water Dominant Stream

OPTIMUM OPERATING CONDITIONS FOR DISTILLATION COLUMN

- Goal: **Maximize styrene yield and purity by optimizing the number of stages in the distillation column.**
- Number of Stages: **Simulation results show that 50–52 stages yield the highest styrene purity with minimized ethylbenzene presence. Increasing stages beyond this point adds cost without improving purity.**
- Temperature Profile: **The temperature at the selected stages (~140°C) aligns with styrene's boiling point (~145°C), allowing for effective separation from ethylbenzene (boiling point ~135°C).**

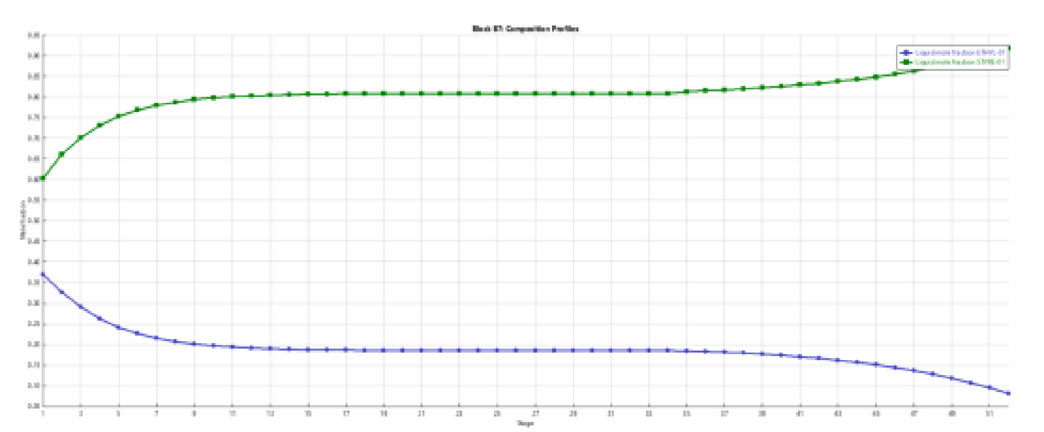


Fig-6 Mole fraction versus Number of Stages in Distillation Column

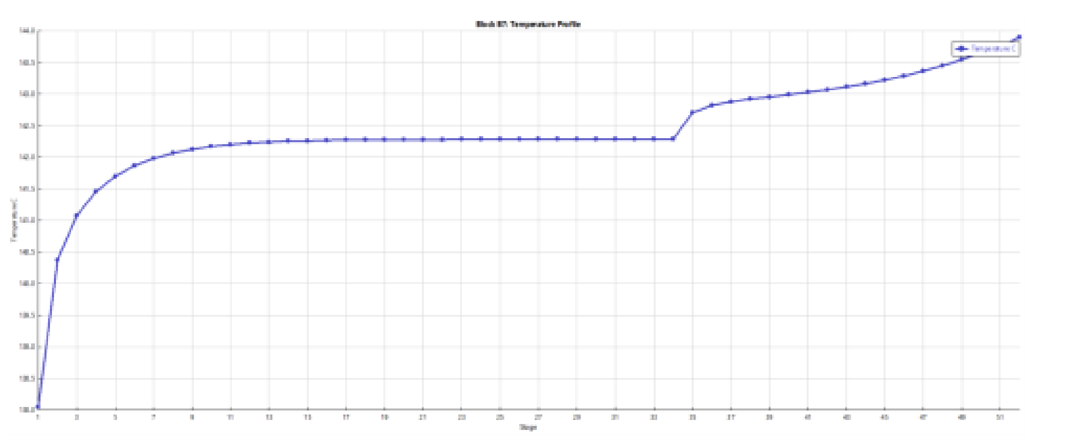


Fig-7 Temperature Profile in Distillation Column

CATALYSTS

Catalysts

1. Iron-Based Catalysts
2. Noble Metal Catalysts
3. Nickel-Based Catalysts

CATALYSTS

Iron-Based Catalysts

- Description: Widely used in the industry, often supported on silica or alumina.
- Advantages: High activity at operational temperatures (600–620 °C), good selectivity towards styrene with minimal by-products.
- Cost: Inexpensive, around $1–$3 per kg.

Noble Metal Catalysts (e.g., Platinum, Palladium)

- Description: Highly effective but rarely used for styrene due to high costs.
- Advantages: Extremely high activity and selectivity, potential for lower operational temperatures.
- Disadvantages: Very high cost, making them impractical for large-scale applications.
- Cost: $20,000–$60,000 per kg, significantly more expensive than iron.

Nickel-Based Catalysts

- Description: Used in various catalytic processes but less common for ethylbenzene dehydrogenation.
- Advantages: Moderate cost and reasonable activity.
- Disadvantages: Lower selectivity towards styrene and prone to deactivation by coking.
- Cost: $5–$10 per kg, more affordable than noble metals but higher than iron.

ENVIRONMENTAL IMPACT

Vent gas emissions and wastewater discharges associated with this process present significant environmental and health risks, including climate change, air pollution, water contamination, and toxicity to both humans and wildlife.

VENT GAS ANALYSIS

The vent gas stream primarily consists of Methane, Hydrogen, and Ethylbenzene,each each posing specific environmental and health risks

METHANE
A potent greenhouse gas, methane has a global warming potential over 25 times greater than CO_2. It contributes to climate change, worsens air quality by forming ground-level ozone, and poses explosion risks in confined spaces.

HYDROGEN
While hydrogen itself is clean, its production from natural gas (through steam methane reforming) can release CO_2, contributing to greenhouse gas emissions.

ETHYLBENZENE
A volatile organic compound (VOC), ethylbenzene contributes to air pollution, and chronic exposure can cause respiratory issues and is a potential carcinogen.

WATER ANALYSIS

The upper distillation column contains a mixture of Benzene, Toluene, and water, posing serious risks to aquatic ecosystems and human health:

BENZENE

A known carcinogen, it is toxic to both humans and aquatic life.
Discharging benzene into water bodies can lead to contamination and bioaccumulation in the food chain.

TOLUENE

Neurotoxic, it can cause headaches, dizziness, and long-term neurological damage. It also harms aquatic organisms and disrupts ecosystems when discharged into water.

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Conclusion

- Successful Mini-Plant Simulation: Completed a simulation for styrene production from ethylbenzene, achieving efficient dehydrogenation and effective separation using an isothermal reactor and distillation column.
- Optimization Achievements: Identified optimal conditions for the LLV separator and distillation column, improving product yield and reducing unwanted by-products. Iron-based catalysts were selected for cost-efficiency and high selectivity.
- Environmental Impact: Addressed the environmental risks posed by vent gases (e.g., methane, hydrogen) and wastewater containing benzene and toluene. Highlighted the need for effective emission control and water treatment.

Future work

- Advanced Catalyst Testing: Explore catalysts beyond iron, like more affordable alternatives with higher activity, to further boost efficiency and reduce energy consumption.
- Enhanced Emission Controls: Implement advanced vent gas and wastewater treatment technologies to mitigate environmental impacts.
- Scale-Up Studies: Evaluate the scalability of the mini-plant process for industrial applications, focusing on maintaining efficiency and environmental compliance at larger scales.

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THANK YOU

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