CHE654 Design Project #4

Semester 1, 2025

🧩 Problem Statement

Project Title

Simulation and Economic Evaluation of Phenol Production from Benzene and Propylene via the Cumene Process Using Aspen Plus

---

Background

Phenol (C_6H_5OH) is an essential industrial chemical used in the production of **bisphenol A**, **caprolactam**, **phenolic resins**, and other derivatives. The dominant industrial method for phenol production is the **Hock process**, where **benzene and propylene** react to form **cumene**, which is then oxidized to **cumene hydroperoxide** and subsequently cleaved to produce **phenol and acetone**.

This project aims to simulate the phenol production process in **Aspen Plus**, analyze its technical feasibility via mass and energy balances, and assess the **economic viability** through financial indicators such as **IRR, NPV, and payback period**.

Objectives

1. Simulate the production of **phenol** from **benzene and propylene** through the **cumene (Hock) process** using **Aspen Plus**.
2. Develop a **detailed process flow diagram (PFD)** including all major unit operations.
3. Perform **material and energy balances** to determine process efficiency.
4. Generate **stream tables** and key **operating parameters** for simulation units.
5. Conduct an **economic evaluation** using:
    - **Internal Rate of Return (IRR)**
    - **Net Present Value (NPV)**
    - **Payback Period**
    - **Cash Flow Analysis**
6. Evaluate the **financial viability** of the process and provide recommendations for scale-up or optimization.

🔬 Process Description

Main Reaction Steps:

1. Alkylation:

C_6H_6 (benzene) + C_3H_6 (propylene) → $C_6H_5CH(CH_3)_2$ (cumene)

2. Oxidation:

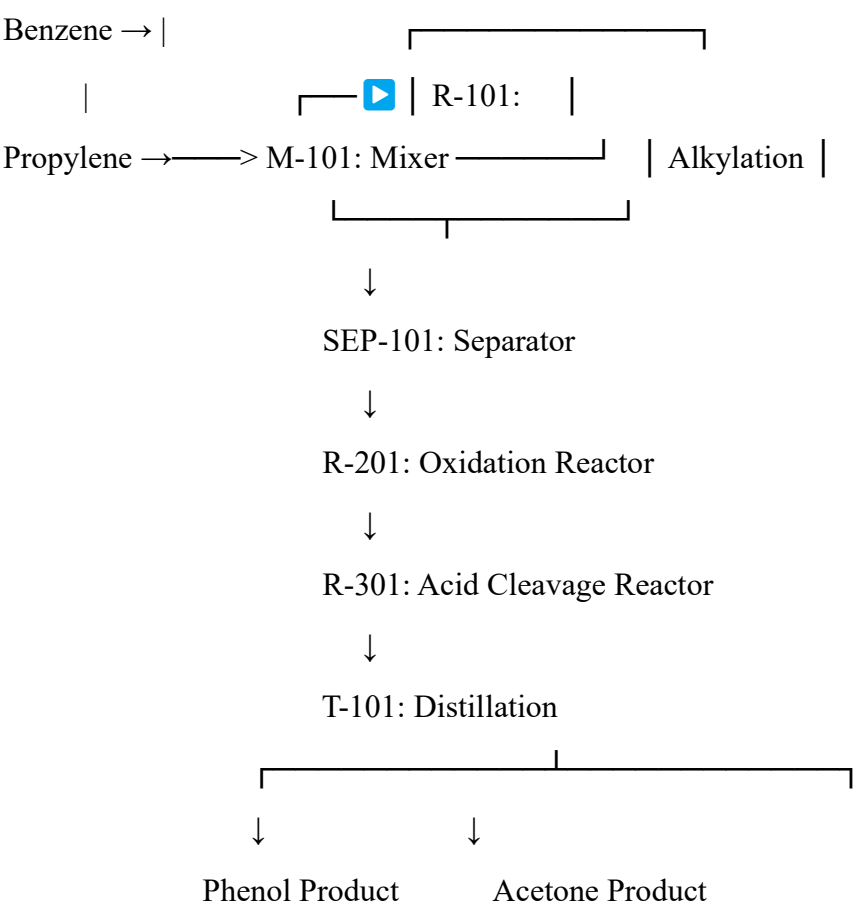
$C_6H_5CH(CH_3)_2 + O_2 \rightarrow C_6H_5C(CH_3)_2OOH$ (cumene hydroperoxide)

3. Cleavage (Acid-Catalyzed):

$C_6H_5C(CH_3)_2OOH \rightarrow C_6H_5OH$ (phenol) + CH_3COCH_3 (acetone)

- **Byproducts**: α-methylstyrene, acetophenone, and tars (in small amounts)

📐 Conceptual Process Flow Diagram (PFD)



📜 Aspen Plus Simulation Setup

1. Thermodynamic Model

- Use **Peng-Robinson (PR)** or **NRTL** for handling non-ideal liquid/vapor behavior.
- Use **RK-Aspen** or **SRK** for initial approximations in hydrocarbon systems.

---

2. Components

Component	Formula	Role
Benzene	C_6H_6	Feed
Propylene	C_3H_6	Feed
Cumene	C_9H_{12}	Intermediate
Cumene Hydroperoxide	$C_9H_{12}O_2$	Intermediate (in Aspen: may require hypothetical compound)
Phenol	C_6H_5OH	Product
Acetone	CH_3COCH_3	Co-product
Oxygen	O_2	Oxidant
Water, N_2	Miscellaneous	Side products / purge gases

---

3. Typical Operating Conditions

Unit	Temperature (°C)	Pressure (bar)	Description
Alkylation	200–250	20–30	Acid catalyst (e.g., zeolite or phosphoric acid)
Oxidation	100–140	3–6	Air/O_2 bubbled through cumene
Cleavage	50–80	~1–2	H_2SO_4 catalyst used
Distillation	80–200	~1	Separation of phenol, acetone

📊 Input Data for Aspen Simulation

A. Feed Data (Example Basis)

Component	Flowrate (kmol/h)	Purity (%)	Source
Benzene	100	99.9	Purchased
Propylene	100	99.5	Purchased
Air/O_2	150	21% O_2	Utility
Catalyst	-	Fixed bed	Reactor input only

These values can be scaled depending on target phenol production (e.g., 10,000–50,000 TPA).

💰 Economic Evaluation Framework

A. Capital Expenditure (CapEx)

- Reactor vessels (alkylation, oxidation, cleavage)
- Separators and distillation columns
- Heat exchangers, pumps, and utilities
- Catalyst loading and infrastructure
- Contingency and installation

B. Operating Expenditure (OpEx)

- Raw materials (benzene, propylene, air)
- Catalyst replacement
- Utilities: steam, cooling water, electricity
- Labor, maintenance, and waste handling

C. Financial Indicators

Metric	Purpose
IRR	Return rate based on project cash flows
NPV	Net present value over project life
Payback Period	Time to recover initial investment
Cash Flow	Annual revenue minus expenses over time

D. Economic Assumptions (Example)

Parameter	Value
Project Life	15–20 years
Discount Rate	10%
Construction Time	2 years
Operating Days/year	330
Plant Capacity	20,000–50,000 TPA
Depreciation	Straight-line (10 yrs)

✅ **Deliverables**

1. **Aspen Plus Simulation File (.bkp)**
    - Material & energy balance, flowsheets
2. **Process Flow Diagram (PFD)**
3. **Stream Tables & Equipment List**
4. **Utility & Catalyst Consumption Estimates**
5. **Economic Model (Excel/Spreadsheet)**:
    - IRR, NPV, Payback, Cash Flows
6. **Report Summary**:
    - Technical description
    - Economic conclusions
    - Sensitivity analysis (raw material price, scale, utility cost)
