PROJECT: Energy - Efficient Process Design and Simulation for Cumene Production

CL317: Process Synthesis, Design, and Simulation

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Contents

1 Introduction

Cumene (isopropylbenzene) is a crucial intermediate in the chemical industry, primarily used in the production of phenol and acetone. These chemicals are essential raw materials for a wide range of products, including plastics, resins, adhesives, and solvents. The global demand for cumene continues to grow, driven by the increasing need for phenol-based products in various industries such as automotive, construction, and electronics. As a result, the development of efficient and sustainable cumene production processes is of significant industrial importance.

The conventional method for cumene production involves the alkylation of benzene with propylene, catalyzed by an acid catalyst. This process typically yields cumene along with by-products such as p-diisopropylbenzene (p-DIPB). While the process is well-established, there is a growing need to optimize it for better resource utilization, energy efficiency, and environmental sustainability. To address these needs, this project focuses on designing an energy-efficient and sustainable cumene production process by integrating advanced process design techniques, heat recovery strategies, and waste minimization methods. Using process simulation tools like Aspen Plus and MATLAB, the behavior of the reactor and separation systems can be studied in detail to improve performance.

The main chemical reactions involved in the process are as follows:

$$\underbrace{C_3H_6}_{\text{Propylene}} + \underbrace{C_6H_6}_{\text{Benzene}} \xrightarrow{\text{Catalyst}} \underbrace{C_9H_{12}}_{\text{Cumene}} \quad \text{(Desired)}$$

$$\underbrace{C_3H_6}_{\text{Propylene}} + \underbrace{C_9H_{12}}_{\text{Cumene (or Trimethylbenzene)}} \xrightarrow{\text{Catalyst}} \underbrace{C_{12}H_{18}}_{\text{Diisoprpyl Benzene}} \quad \text{(Undesired)}$$

1.1 Motivation

This project is motivated by several key factors influencing the modern chemical process industry:

1. **Energy Efficiency Imperatives:** Chemical processes account for approximately 10% of global energy consumption, with significant potential for improvement through efficient design. The cumene production process, specifically, involves energy-intensive separation steps that can benefit substantially from optimization.

2. **Environmental Sustainability:** Regulatory pressures and corporate sustainability goals increasingly demand processes with reduced environmental footprints. Minimizing waste streams, reducing emissions, and improving resource utilization are critical considerations in modern process design.

3. **Economic Competitiveness:** With razor-thin margins in commodity chemical production, even small improvements in yield, selectivity, or en-

ergy consumption can translate to significant economic advantages. Process optimization directly impacts the economic viability of production facilities.

4. **Technological Advancement:** Innovations in catalysis, separation technologies, and process control offer new opportunities to enhance established processes. Leveraging these advances can lead to step-change improvements in process performance.

Objectives

The primary objectives of this project are as follows:

- To design a complete process for the production of Cumene from Benzene and Propylene using Aspen Plus simulation.
- To perform a detailed material and energy balance for the process.
- To select and design major equipment involved in the production process, including the reactor, distillation columns, and heat exchangers.
- To analyze the economic feasibility of the proposed process through capital and operating cost estimation.
- To ensure environmental and safety considerations are integrated into the process design.

2 System Description

The following flowsheet represents a chemical process involving the separation and reaction of hydrocarbons, specifically benzene and propane. The system consists of essential unit operations, including a separator, heat exchanger, reactor, and various process streams, ensuring efficient processing and conversion.

The final cumene production process involves the alkylation of benzene with propylene to form cumene, with minor by-products such as p-diisopropylbenzene (p-DIPB). The process was developed incrementally in three stages – starting with a basic configuration, then adding a recycle stream, and finally incorporating heat integration. Each stage focused on improving conversion, resource utilization, and energy efficiency. The final flowsheet employs several unit operations such as mixers, vapor-liquid separators, heat exchangers, a plug flow reactor, a flash separator, pumps, and distillation columns.

2.1 Initial Process Design (Without Recycle or Product Separation)

In the base design, the process begins with the fresh introduction of reactants and proceeds through core reaction and separation steps without any recycle or product separation.

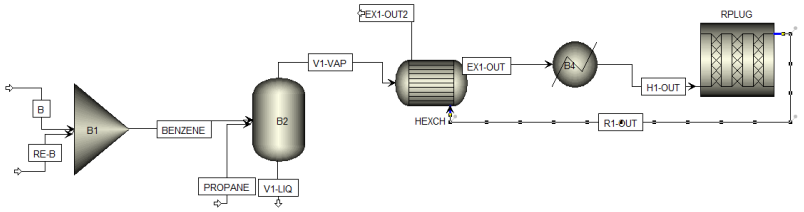

Figure 1: Process Flow Diagram

- **Feed Introduction and Flash Separation:** Fresh benzene and propylene streams are introduced into a flash separator (FLASH). The purpose of this flash unit is to perform a preliminary separation under high pressure. The vapor phase (V1-VAP), primarily containing benzene and propylene, continues forward.
- **Preheating and Reaction:** The vapor stream is first passed through a heat exchanger (HEATX), where it is preheated using energy recovered from the downstream reactor outlet. It is then further heated using an external heater (HEATER) to reach the required reaction temperature (345°C). The stream enters an adiabatic plug flow reactor (RPLUG) where the primary reaction occurs: benzene and propylene react to form cumene, with a small amount of p-DIPB as a side product.
- **Stream Exit:** In the base design, the process ends at the reactor outlet (R1-OUT) after passing through the heat exchanger (HEX). No cooling, separation, or product recovery units are included at this stage.

2.2 Enhanced Design with Recycle, Product Separation

The next stage of process development introduced a recycle structure and downstream separation units to improve raw material utilization and enable product purification.

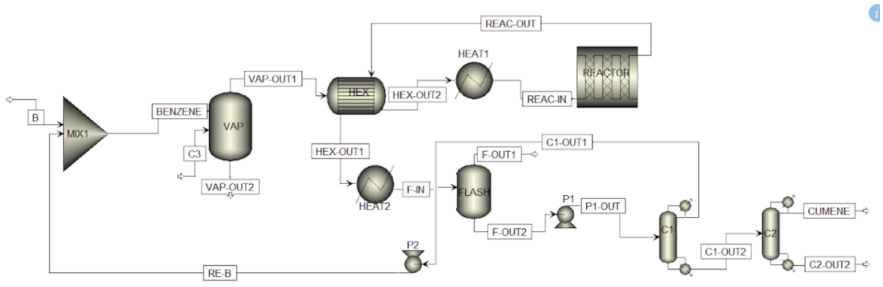

Figure 2: Process Flow Diagram

- **Recycle Loop:** The top product from the first distillation column (C1-OUT1), containing unreacted benzene, is recycled back to the beginning of the process. This recycled benzene is combined with fresh benzene in a newly introduced mixer (MIX1). The mixed benzene stream is then sent to the flash separator (VAP) as the new process starting point.
- **Propylene Addition:** After flash separation, propylene is introduced into the vapor stream (F-OUT1) before entering the HEX and HEAT1, maintaining correct stoichiometry and minimizing the potential for over-alkylation.
- **Post-Reaction Cooling and Flash Separation:** The reactor outlet (REAC-OUT) is cooled by transferring its heat back to the incoming feed via HEX, and further cooled using HEAT2. The cooled stream is sent to a flash separator (FLASH), where: **F-OUT1:** A vapor stream containing light gases like unreacted propylene and propane is removed. **F-OUT2:** A liquid stream containing benzene, cumene, and DIPB proceeds to separation.
- **Product Separation:** The liquid stream is pumped by P1 into the first distillation column (C1), which separates benzene (top product, C1-OUT1) for recycling, and sends cumene + DIPB as the bottom product (C1-OUT2) to C2. The second column (C2) separates cumene as the top product (C2-OUT1) and removes DIPB as the bottom product (C2-OUT2).

2.3 Key Components and their properties

Property	Benzene	Propylene	Propane	Cumene	p-DIPB
Formula	C_6H_6	C_3H_6	C_3H_8	C_9H_{12}	$C_{12}H_{18}$
State at 25°C & 1 atm	Liquid	Gas	Gas	Liquid	Liquid
Boiling Point (°C)	80.08	−47.7	−42.11	152.4	210.3
Density (g/cm³ at 20°C)	0.8788	0.001 78	0.001 8	0.8615	0.8568
Critical Temperature (°C)	288	99.2	91.44	358	521
Molecular Weight (g/mol)	78.122	42.08	44.096	120.191	162.271
Thermal Conductivity (W/m·°C at 25°C)	0.131	0.017	0.018	0.132	0.1555
Formula	C_6H_6	C_3H_6	C_3H_8	C_9H_{12}	$C_{12}H_{18}$
Critical Pressure (kPa)	4852	4239	4579	3210	9778
Vapor Pressure (kPa at 25°C)	12.7	1159	939	0.61	0.037
Melting Point (°C)	5.538	−185.17	−187.7	−96.01	−17.1

Table 1: Physical and Chemical Properties of the key Components

2.4 Flowsheet Parameters

Flash Separators (Flash2)	Temp (°C)	Pressure (bar)
VAP	210	25.00
FLASH	90	1.75

Table 2: Operating Conditions for Flash Separators

Heaters	Temp (°C)	Pressure (bar)
HEAT1	345	25.00
HEAT2	90	1.75

Table 3: Operating Conditions for Heaters

Pump	P1 Pressure (bar)	P2 Pressure (bar)
Discharge Pressure	1.78	25

Table 4: Operating Conditions for Pumps

Heat Exchanger (HEATX)	**Value**
Unit's Name	HEX
Model Fidelity	Shortcut
Flow Direction	Counter Current
Cold Stream Outlet Temp (°C)	330
Min. Temp Approach (°F)	1.8

Table 5: Specifications of Heat Exchanger (HEATX)

RADFRAC	**C1**	**C2**
Total Stages	15	20
Reflux Ratio	0.44	0.62
Bottoms Rate (kmol/hr)	94.81	1.952
Feed Stage	8 (On-Stage)	11 (On-Stage)
Stage 1 Pressure (bar)	1.75	1.00
Stage 20 Pressure (bar)	–	1.00

Table 6: RADFRAC Column Specifications

Reactor (RPLUG)	**Value**
Unit's Name	RPLUG
U ($kW/m^2 \cdot K$)	0.065
Thermal Fluid Temperature (°C)	360
Number of Tubes	340
Length (m)	6
Diameter (m)	0.0765
Bed Voidage	0.5
Particle Density (kg/m^3)	1900

Table 7: Plug Flow Reactor (RPLUG) Parameters

Feed Specifications	Benzene Feed (B)	Propylene Feed (C3)
Temperature (°C)	25	25
Pressure (bar)	25	25
Total Flowrate (kmol/hr)	104.2	110
Mole Fraction (Benzene)	1.00	0.00
Mole Fraction (Propane)	0.00	0.05
Mole Fraction (Propylene)	0.00	0.95

Table 8: Feed specifications for Benzene and Propylene streams

3 Methodology

NRTL RK was used in aspen while for verification mass and energy balance equations for the control volume were use which are defined below:

3.1 RPLUG Mass and Energy Balance

The PFR design equation for a reactant A at steady-state is given by:

$$\frac{dF_A}{dV} = r_A \tag{1}$$

where:

- F_A : Molar flow rate of A (mol/s)
- V : Reactor volume (m^3)
- r_A : Rate of reaction of A ($mol/m^3 \cdot s$)

Since the rate of reaction is given by:

$$r_A = -kC_A \tag{2}$$

Substituting concentration C_A as:

$$C_A = \frac{F_A}{v} \tag{3}$$

where v is the volumetric flow rate, we get:

$$\frac{dF_A}{dV} = -k\frac{F_A}{v} \tag{4}$$

Integrating over the reactor volume:

$$\int_{F_{A0}}^{F_A} \frac{dF_A}{F_A} = -\frac{k}{v}\int_0^V dV \tag{5}$$

Solving the integral,

$$\ln\left(\frac{F_A}{F_{A0}}\right) = -\frac{kV}{v} \tag{6}$$

which simplifies to:

$$F_A = F_{A0}e^{-\frac{kV}{v}} \tag{7}$$

V is calculated as:

$$V = N_{tubes} \times L \times A_{tube} \tag{8}$$

where:

- N_{tubes} : Number of tubes
- L : Tube length
- A_{tube} : Tube cross-sectional area

  For the series of reactions:

$$C_3H_6 + C_6H_6 \rightarrow C_9H_{12} \quad (A + B \rightarrow C) \tag{9}$$
$$C_3H_6 + C_9H_{12} \rightarrow C_{12}H_{18} \quad (A + C \rightarrow D) \tag{10}$$

The design equations are:

$$\frac{dF_A}{dV} = -(k_1C_AC_B + k_2C_AC_C) \tag{11}$$
$$\frac{dF_B}{dV} = -k_1C_AC_B \tag{12}$$
$$\frac{dF_C}{dV} = k_1C_AC_B - k_2C_AC_C \tag{13}$$
$$\frac{dF_D}{dV} = k_2C_AC_C \tag{14}$$

The reaction rate constants k_1 and k_2 are given by the Arrhenius equation:

$$k_1 = A_1 \exp\left(\frac{-E_{a1}}{RT}\right)$$

$$k_2 = A_2 \exp\left(\frac{-E_{a2}}{RT}\right)$$

where:

- A_1, A_2 are the pre-exponential factors,
- E_{a1}, E_{a2} are the activation energies (J/mol),
- R is the universal gas constant (J/mol.K),
- T is the temperature in Kelvin.

3.2 Energy Balance Equation

The general **steady-state energy balance** for an adiabatic reactor is:

$$\frac{dT}{dV} = \frac{-\sum(-\Delta H_r)r_i}{F_{total}C_p} \tag{15}$$

where:

- ΔH_r = Heat of reaction (kJ/mol)
- r_i = Reaction rate (mol/m^3·s)
- F_{total} = Total molar flow rate (kmol/s)
- C_p = Heat capacity (J/mol·K)

The equations are solved in MATLAB using ode solver for each value of PFR volume element.

3.3 Flash Calculations

After the reactor output is cooled, the stream contains five main components: propylene, propane, benzene, cumene, and DIPB. Given the significantly lower boiling points of propane and propylene, a flash separator (Flash2, V802) is employed to separate the vapor-phase light components (C hydrocarbons) from the heavier components (aromatics). The separation is based purely on phase equilibrium at the specified temperature and pressure.

Assumptions:

- The flash operates at 90°C and 1.75 bar.
- Propylene and propane are assumed to fully vaporize and exit with the vapor stream.
- Benzene, cumene, and DIPB remain entirely in the liquid stream.
- No chemical reaction occurs during the flash separation; the process is isothermal and isobaric.

Mass Balance Equations:

$$F_{\text{in}} = F_{\text{out-1, vapor}} + F_{\text{out-2, liquid}}$$

$$F_{\text{propylene}} + F_{\text{propane}} = F_{\text{out-1, vapor}}$$

$$F_{\text{benzene}} + F_{\text{cumene}} + F_{\text{DIPB}} = F_{\text{out-2, liquid}}$$

This separation allows the light gases to be purged or recycled, while the heavier aromatics proceed to further purification via distillation.

3.4 Distillation Column 1 (C1) - Benzene Recovery

The liquid output from the flash separator is sent to the first distillation column (RADFRAC C1), which is designed to recover benzene from the cumene and DIPB mixture.

Assumptions:

- The distillation column operates with 15 stages and a feed at stage 8.
- Operating pressures: Top = 1.75 bar.
- Benzene is highly volatile and is assumed to be separated with 99.9% purity in the top product.
- Cumene and DIPB, being less volatile, are assumed to remain in the bottom product.

Mass Balance for Benzene:

$$F_{\text{benzene, top}} = \xi_{\text{benzene}} \cdot F_{\text{benzene, in}}$$

$$F_{\text{benzene, bottom}} = (1 - \xi_{\text{benzene}}) \cdot F_{\text{benzene, in}} \approx 0$$

Overall Bottoms Stream:

$$F_{\text{bottoms}} = F_{\text{cumene}} + F_{\text{DIPB}} + (1 - \xi_{\text{benzene}}) \cdot F_{\text{benzene}} \approx F_{\text{cumene}} + F_{\text{DIPB}}$$

The benzene recovered from the top stream is routed back to the reactor as part of the recycle loop to enhance process efficiency and reduce raw material losses.

3.5 Distillation Column 2 (C2) – Cumene Recovery

In this second distillation column (RADFRAC C2), the *bottom product* from Distillation Column 1 (C1) (which mainly contains cumene and DIPB, with only trace amounts of benzene) is fed at a specified stage. The primary objective is to achieve high purity cumene inphtop product, while DIPB (and any remaining heavy components) exit in product. A typical design goal here is to separate cumene with at least 99.9% purity overhead.

Assumptions:

- The distillation column operates with 20 stages (including a reboiler and a total condenser).
- The feed enters at stage 11.
- The operating pressure at the top of the column is assumed to be **1 bar**.
- Cumene, which is more volatile than DIPB, is assumed to achieve **99.9**% purity in the top product.
- DIPB and any other heavier components remain in the bottom product.

Mass Balance for Cumene: Since cumene is predominantly recovered overhead, the majority of Cumene from the feed (F_{cumene}) appears in the top distillate stream. Only a small fraction (due to incomplete separation or non-idealities) may remain in the bottoms. We can write a simplified overall balance:

$$F_{\text{cumene, feed}} = D_{\text{cumene, top}} + B_{\text{cumene, bottom}},$$

where

- $F_{\text{cumene, feed}}$ is the total Cumene in the feed to C2,
- $D_{\text{cumene, top}}$ is the amount of Cumene recovered in the overhead product,
- $B_{\text{cumene, bottom}}$ is the small fraction of Cumene lost to the bottoms.

With a 99.9% overhead recovery assumption for cumene,

$$D_{\text{cumene, top}} \approx 0.999 \times F_{\text{cumene, feed}}.$$

Overall Bottoms Stream: The bottoms stream from C2 is dominated by DIPB. A simplified material balance for DIPB can be written as:

$$F_{\text{DIPB, feed}} = D_{\text{DIPB, top}} + B_{\text{DIPB, bottom}},$$

but because DIPB is much less volatile, we assume

$$D_{\text{DIPB, top}} \approx 0,$$

and thus

$$B_{\text{DIPB, bottom}} \approx F_{\text{DIPB, feed}}.$$

Under these assumptions, almost all of the DIPB leaves via the reboiler, while nearly all Cumene appears in the overhead distillate. Any small benzene or other lights that might have entered the feed will likely exit in the top product, given their higher volatility relative to those of Cumene and DIPB.

4 Results

Stream	C1-OUT1	C1-OUT2	C2-OUT2	CUMENE	F-IN	F-OUT1	F-OUT2	REAC-IN	REAC-OUT
Temperature (°C)	41.51	175.86	209.22	151.80	90	90	90	345	423.39
Pressure (bar)	1.75	1.75	1	1	1.75	1.75	1.75	25	25
Mole Flow (kmol/h)	87.52	100.47	3.05	97.42	197.79	9.79	187.99	301.72	197.79
BENZENE	79.05	0.0603	1.43×10^{-13}	0.0603	82.38	3.28	79.11	183.25	82.38
PROPANE	6.99	4.73×10^{-9}	1.14×10^{-26}	4.73×10^{-9}	12.49	5.50	6.99	12.49	12.49
PROPY-01	0.724	5.14×10^{-10}	5.43×10^{-28}	5.14×10^{-10}	1.29	0.567	0.724	105.22	1.29
ISOPR-01	0.759	97.35	0.000 035	97.35	98.55	0.447	98.11	0.759	98.55
P-DII-01	3.98×10^{-8}	3.07	3.05	0.014	3.07	0.0016	3.07	3.98×10^{-8}	3.07

Table 9: Stream data including temperature, pressure, and mole flows of components

The stream data presented in Table above confirms the successful operation of the entire cumene production process, including feed preparation, reaction, separation, and recycle. The reactor inlet stream (REAC-IN) consists predominantly of benzene and propylene with mole flows of 183.25 kmol/h and 105.22 kmol/h respectively, consistent with stoichiometric feed ratios.

At the reactor outlet (REAC-OUT), benzene and propylene decrease significantly to 82.38 kmol/h and 12.49 kmol/h, indicating substantial conversion. The formation of 98.55 kmol/h of cumene and 3.07 kmol/h of DIPB validates the reaction's effectiveness. The presence of propane in the outlet is attributed to impurity in the propylene feed (5% propane), which remains unreactive and is carried through the system.

The top and bottom products of the first distillation column (C1) also support the recovery and recycle strategy: 79.05 kmol/h of benzene is efficiently recovered in the top stream (C1-OUT1), with only 0.0603 kmol/h present in the bottoms, indicating a high separation efficiency. Similarly, C2-OUT1 contains the bulk of the cumene (97.35 kmol/h), with minimal DIPB impurity, while DIPB is mostly directed to C2-OUT2.

```
PFR mass and energy balance
FA (Propylene) = 13.6800 kmol/h
FB (Benzene) = 81.0929 kmol/h
FC (Cumene) = 100.2727 kmol/h
FD (DIPB) = 1.88148035 kmol/h
T_end = 421.8713 deg C
```

Figure 3: Outlet Mole Flows from PFR

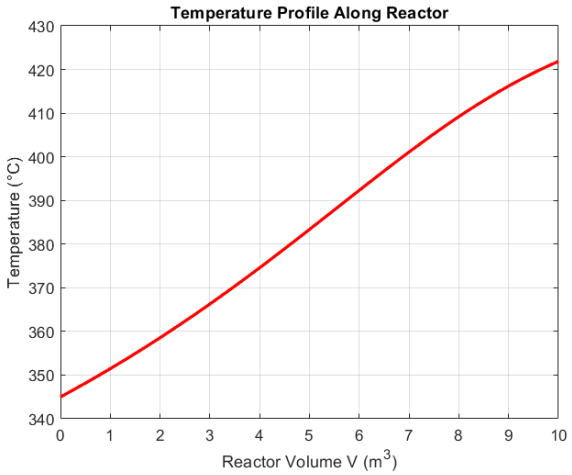

Figure 4: Temperature profile along the reactor volume

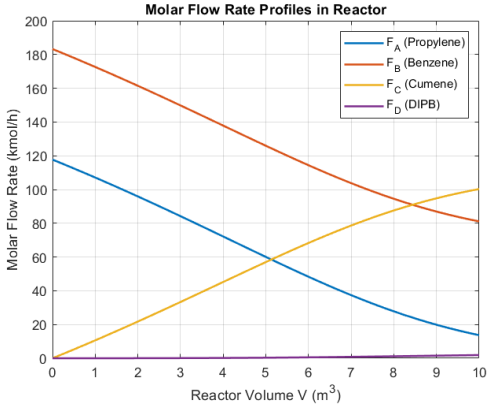

Figure 5: Mole flowrate profile

Component / Property	**REAC-OUT (kmol/h)**	**PFR Output (kmol/h)**	**Error (%)**
Propylene (C3)	12.4920	13.6800	9.51
Benzene (B)	82.3840	81.0929	1.57
Cumene (C)	98.5531	100.2727	1.74
DIPB (D)	3.0689	1.8815	38.70
Temperature (°C)	423.3937	421.8713	0.36

Table 10: Comparison of REAC-OUT stream and PFR output

Stream	Flash Balance (kmol/h)	Flash Output (Aspen) (kmol/h)	Error (%)
Top Product (Propane + Propylene)	13.6800	9.7932	39.7
Bottom Product (Benzene + Cumene + DIPB)	183.2471	187.9964	2.5

Table 11: Comparison of Flash mass balance and Aspen Flash Output

The comparison in Table above shows that the MATLAB-based plug flow reactor (PFR) model closely approximates the Aspen simulation results for major components. Benzene and cumene display errors of just 1.57% and 1.74% respectively. However, the DIPB deviation is significant at 38.70%, which may be attributed to secondary reaction kinetics and assumptions in rate constants used in the MATLAB model. Since DIPB formation is a secondary reaction, even small inaccuracies in residence time or temperature gradient modeling can disproportionately affect its prediction.

For the flash separator, the top product (light gases) shows a significant 39.7% error between the hand calculation and Aspen output, while the bottom product differs by only 2.5%. The discrepancy likely arises due to idealized assumptions in the hand calculation, such as complete vaporization of light components and perfect liquid retention of aromatics. In Aspen, rigorous thermodynamic models capture partial vaporization and real component interactions, leading to a more accurate phase split.

```
Mass balance on 1st Distillation column (C1)

Mole flows in Distillate:
BENZENE:    81.011767 kmol/h
CUMENE:   0.100273 kmol/h
DIPB:   0.000000 kmol/h

Mole flows in Bottom:
BENZENE:    0.081093 kmol/h
CUMENE:   100.172470 kmol/h
DIPB:   1.881480 kmol/h
```

Figure 6: Results from 1st Distillation Column

```
Mass balance on 2nd Distillation column (C2)

Mole flows in Distillate:
BENZENE:    0.081093 kmol/h
CUMENE:   100.072298 kmol/h
DIPB:   0.001881 kmol/h

Mole flows in Bottom:
CUMENE:   0.100172 kmol/h
DIPB:   1.879599 kmol/h
```

Figure 7: Results from 2nd Distillation Column

Stream	Component	Aspen (kmol/h)	MATLAB (kmol/h)	Error %
C1 Top	BENZENE	79.047	81.011767	2.49
	CUMENE	0.7589	0.100273	86.79
	DIPB	3.98E-08	0.000000	0.00
C1 Bottom	BENZENE	0.06028	0.081093	34.49
	CUMENE	97.347	100.172470	2.90
	DIPB	3.067	1.881480	38.65
C2 Top	BENZENE	0.06028	0.081093	34.52
	CUMENE	97.34675054	100.072298	2.799
	DIPB	0.01404978341	0.001881	87.24
C2 Bottom	CUMENE	0.0003053365565	0.100172	327.19
	DIPB	3.053297679	1.879599	38.45

Table 12: Comparison of Distillation Column Streams

The table above illustrates the effective separation achieved in both distillation columns. In Column C1, benzene is recovered with 99.9% purity in the overhead stream (C1-OUT1), while cumene and DIPB are directed to the bottom. MATLAB results show a minor discrepancy in benzene purity (2.49% error), which is within acceptable simulation bounds given the simplifications in distillation modeling.

Column C2 effectively isolates cumene in the overhead and DIPB in the bottom stream. Cumene purity in C2-OUT1 is high (over 97.3% in Aspen), with a marginal presence of DIPB. However, the MATLAB prediction shows significant deviation in DIPB concentrations across both top and bottom products—up to 87.24% error for C2-OUT1. This suggests potential inaccuracies in the relative volatility or tray efficiency estimates used in the analytical calculations, reaffirming the value of rigorous simulation tools like Aspen Plus for separation process design.

Despite some numerical discrepancies, the column design is validated as efficient for targeted product recovery. These differences also provide insight

into where model refinement is needed, especially for minor components and secondary by-products.

5 Optimisation

To improve process efficiency, an optimisation study was performed focusing on two key parameters: the **propylene to benzene feed ratio** and the **reactor inlet temperature**. These parameters significantly influence conversion, selectivity, and energy consumption in the plug flow reactor (PFR).

The optimization problem was solved using MATLAB's `fmincon` solver, with a model incorporating detailed reaction kinetics, energy balances, and plug flow reactor (PFR) performance.

The figure below shows the effect of optimizing the benzene-to-propylene ratio and increasing the inlet temperature on reactor performance. The optimal benzene-to-propylene molar ratio was found to be approximately 0.8:1. This excess benzene suppresses the undesired side reaction forming p-DIPB, thereby improving cumene selectivity.

Raising the inlet temperature from 300°C to 450°C resulted in increased reaction rates, with optimised temparature at 359°C shifting the conversion of both benzene and propylene upward. However, further increase beyond 359°C showed diminishing returns due to thermodynamic limitations and the onset of side-product formation.

Figures also Display the reactor's temperature and molar flowrate profiles under optimised conditions. The temperature profile indicates a typical adiabatic PFR rise due to exothermic reaction heat. Molar flowrates show a rapid decline in reactants and corresponding increase in cumene, validating optimal reaction kinetics and favourable conversion.

```
Optimal feed ratio FA0/FB0 = 0.841
  → FA0 = 137.5019 kmol/h, FB0 = 163.4610 kmol/h
Optimal inlet T = 359.00 °C
Objective J (FD-FC) = -113.5383 kmol/h

Oultle Mole Flows:
→ Propylen+Propane (FA) = 2.8088 kmol/h
→ Benzene  (FD) = 35.8195 kmol/h
→ Cumene : FC = 120.5899 kmol/h
→ DIPB  : FD = 7.0516 kmol/h
→ Temperature at end   (T) = 468.0593 deg C
```

Figure 8: Results after optimizing feed ratio and inlet temperature

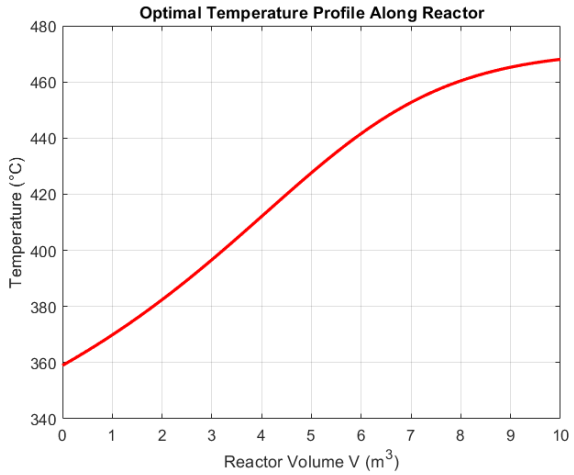

Figure 9: Temperature Profile

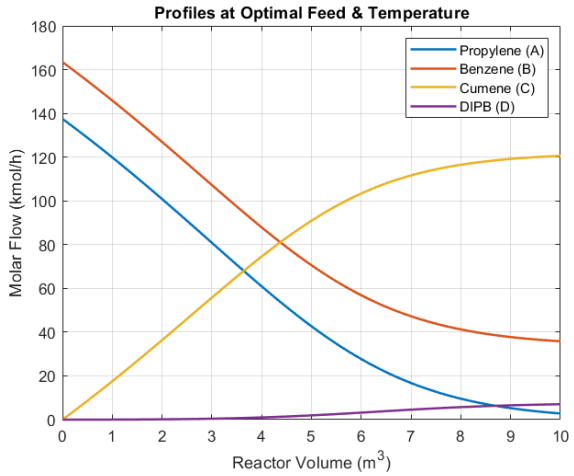

Figure 10: Molar Flowrate Profile

The molar flow profile shows rapid consumption of propylene and benzene, accompanied by the formation of cumene and gradual buildup of DIPB toward the reactor outlet. The temperature profile confirms the exothermic nature of the reactions, with a continuous rise reaching a peak at the reactor exit.

These results form a critical foundation for the subsequent design of downstream separation units and for the implementation of heat recovery strategies to improve the overall process efficiency.

6 Conclusion

This project presents a comprehensive approach to the design, simulation, and optimization of a sustainable cumene production process, integrating fundamental chemical engineering principles with advanced process modeling tools. Through systematic process development in Aspen Plus and MATLAB, we have created a robust and energy-efficient design that optimizes both raw material usage and product purity while minimizing energy consumption and environmental impact.

Integrated Design Success

The project began with a minimal process configuration, where only the reaction step was modeled without recycle or product separation. This provided a baseline for understanding the core reaction dynamics of benzene and propylene alkylation. However, the initial design suffered from low material efficiency, with excess unreacted benzene and no recovery of valuable intermediates.

To address these limitations, an enhanced design was developed that incorporated recycle loops, energy recovery units, and two distillation columns. This final process flowsheet includes:

- A flash separator for light gas removal (propylene and propane).
- Heat integration through a counter-current exchanger.
- Recycle of unreacted benzene to reduce fresh feed demand.
- High-purity product recovery via two RADFRAC distillation columns.

These improvements significantly enhanced material utilization, especially with the efficient recovery of over 99.9% of benzene and 97.3% cumene in the respective columns.

Modeling and Validation

The core reactor behavior was modeled using MATLAB by solving mass and energy balance ODEs for a plug flow reactor. Kinetic expressions for both primary (cumene formation) and secondary (DIPB formation) reactions were implemented, accounting for temperature-dependent rate constants via the Arrhenius equation. The reactor model was validated against Aspen Plus results, showing high agreement for major species such as benzene (1.57% error) and cumene (1.74% error), with some deviation in DIPB predictions (38.7%), likely due to its sensitivity to temperature profiles and secondary reaction kinetics.

Flash separation and distillation were also evaluated analytically and compared with Aspen's rigorous models. While hand-calculated flash output deviated for light gases (up to 39.7% error), this highlighted the importance of using advanced thermodynamic models for phase equilibria.

Process Optimization and Energy Efficiency

A key aspect of this work was the optimization of the reactor inlet temperature and feed ratio using MATLAB. The optimal propylene-to-benzene ratio was determined to be 0.841, with an optimal inlet temperature of 359°C. These conditions resulted in:

- Significant conversion of benzene and propylene in the reactor.
- Increased cumene yield with suppressed formation of the undesired by-product (DIPB).
- Outlet temperatures peaking at 468°C, consistent with exothermic reaction behavior.

Graphical profiles for temperature and component molar flows confirmed the effectiveness of the optimized reactor configuration.

Overall Impact

The final design achieves high efficiency through:

- Improved conversion via optimized reaction conditions.
- Material recovery and recycle integration.
- Energy savings through heat exchange and minimal external heating.
- High-purity cumene production suitable for downstream phenol and acetone synthesis.

The approach demonstrates the successful integration of simulation, reaction engineering, and separation strategies in a unified design framework. While some minor discrepancies were noted between analytical and simulation results—particularly for DIPB and flash vapor splits—these insights serve as a basis for further model refinement and underscore the need for rigorous simulation in industrial-scale design.

In conclusion, this project not only meets its defined objectives but also establishes a scalable, economically viable, and environmentally conscious blueprint for cumene manufacturing. Future enhancements can focus on dynamic control strategies, heat exchanger network optimization, and detailed cost analysis to further improve process performance.

7 Future Work

While the steady-state simulation has provided valuable insights into the design and optimization of the cumene production process, further work can be done to enhance its operability and control. Future extensions of this project may include:

- Implementing **Aspen Dynamics** to study the transient behavior of the process under disturbances and startup/shutdown scenarios. This will allow evaluation of control strategies and process safety under dynamic conditions.
- Utilizing Aspen Plus built-in **optimization tools** (such as sensitivity analysis, economic optimizers, and design spec blocks) to further minimize energy consumption, operating cost, and emissions.
- Integrating advanced **control strategies** (e.g., model predictive control) with the simulation environment to ensure stable operation at optimal conditions.
- Exploring **alternative catalysts and reaction conditions** for improved selectivity and reaction rate.

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