



CHME 400 Capstone Project

Design of a Plant for Industrial Production of Isopropyl Benzene from Benzene and Propylene

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List of abbreviations

Abbreviation	Definition
APEA	Aspen Process Economic Analyzer
API	American Petroleum Institute Standard
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
B	Benzene
CEPCI	Chemical Engineering Plant Cost Index
CIS	Commonwealth of Independent States
DIPB	Diisopropylbenzene
DSTWU	Distillation Winn-Underwood
EBIT	Earnings Before Interest and Taxes
ESI	Electronic Supplementary Information
FAH	High-Flow Alarm
FAL	Low-Flow Alarm
FCI	Fixed Capital Investment
FIC	Flow Indicator Controller
FUG	Fenske-Underwood-Gilliland
GC	Gas Chromatography
HK	Heavy Key
IRR	Internal Rate of Return
ISBL	Inside Battery Limits
LAH	High-Level Alarm
LAL	Low-Level Alarm
LC	Level Controller
LK	Light Key
NPV	Net Present Value
OSBL	Offsite Battery Limits

P	Propylene
PAH	High-Pressure Alarm
PAL	Low-Pressure Alarm
PSV	Pressure Safety Valve
SPA	Solid Phosphoric Acid
TAH	High-Temperature Alarm
TAL	Low-Temperature Alarm
TI	Temperature Indicator
USD	United States Dollar

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Summary

Isopropyl benzene, or cumene, is an aromatic compound commonly used in the petrochemical industry in the production of phenol and acetone. There are many cumene production technologies, with this study primarily focusing on the transalkylation route. This route is characterized by high conversion and reaction yield, as well as low formation of DIPB as a side product. Both alkylation and transalkylation are carried out over a zeolite- β catalyst, which provides superior selectivity toward cumene under design conditions.

In this work, a complete process of cumene production from propylene and benzene was developed. It includes material balance, the choice of kinetic model, and the design of major and minor equipment, namely a heat exchanger, alkylation and transalkylation reactors, distillation columns, heaters, coolers, pumps, and storage tanks. The plant was planned to have a production capacity of approximately 140,000 tonnes of cumene per year and was proposed for Atyrau due to its suitable industrial infrastructure.

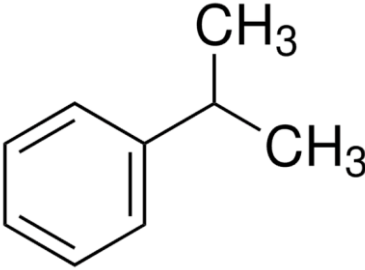
Additionally, the plant layout was designed, and HAZOP analysis and economic evaluation were conducted. Based on the results, the proposed plant meets product demand and is economically feasible.

Chapter 1. Process Introduction

1.1 Physical and Chemical Properties

Cumene (isopropylbenzene) is a colorless, flammable liquid hydrocarbon that serves as a crucial intermediate in the petrochemical industry. It is a type of alkylbenzene and a class of aromatic hydrocarbons with an alkyl group attached to the benzene ring [1]. The main physical properties of cumene are summarized in Table 1.1.1.

Table 1.1.1. Properties of cumene. Data is retrieved from Chemical Book [2]

Properties		Structure
IUPAC Name	Isopropyl benzene	
Molecular Formula	C ₉ H ₁₂	
Appearance	Colorless liquid with gasoline-like odor	
Molecular Weight, g/mol	120.19	
Melting point, K	177.40	
Boiling point, K	425.56	
Density, kg/m ³	861	

1.2 Cumene Applications

The compound is highly valued for its role in the cumene process, where it is converted into cumene hydroperoxide, which is then used to produce phenol and acetone. These derivatives find widespread use in the manufacture of resins, plastics, synthetic fibers, adhesives, and pharmaceuticals, making cumene an essential industrial feedstock.

The main industrial process for producing phenol and acetone is the cumene oxidation process, also known as the Hock Process. The separation of cumene hydroperoxide (CHP) from cumene oxidation products and the demonstration of its acid-catalyzed conversion to 3-phenol and acetone were the first industrial methods of using the cumene. The Process involves two main steps:

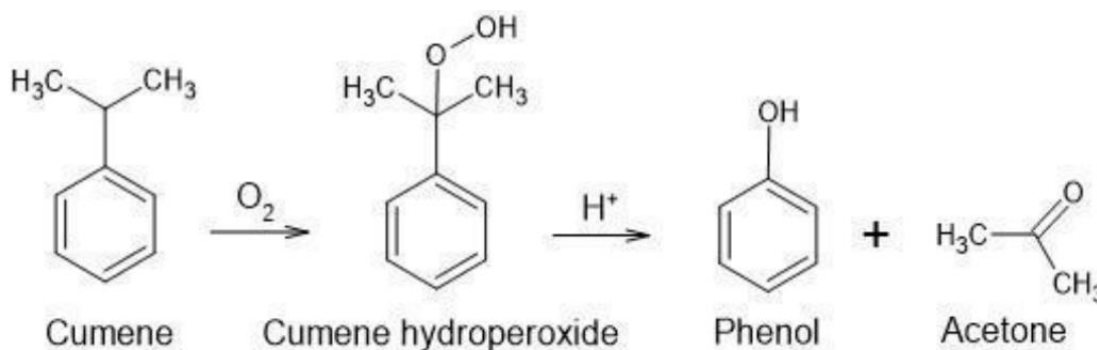


Figure 1.2.1. Production of phenol and acetone from cumene, retrieved from [3]

1.3 Market Analysis

Global demand for cumene was estimated at approximately 17 million metric tons in 2022 [3], with around 95% of cumene consumed for phenol production and roughly 25% used as an acetone co-product [4]. Based on the compound annual growth rate (CAGR) of acetone - estimated at 4.2-5.3% annually - cumene demand is projected to grow at an average rate of approximately 17% per year, bringing global demand to around 27 million metric tons by 2025 and 141 million metric tons by 2035 (see detailed calculations in Appendix B.1) [5].

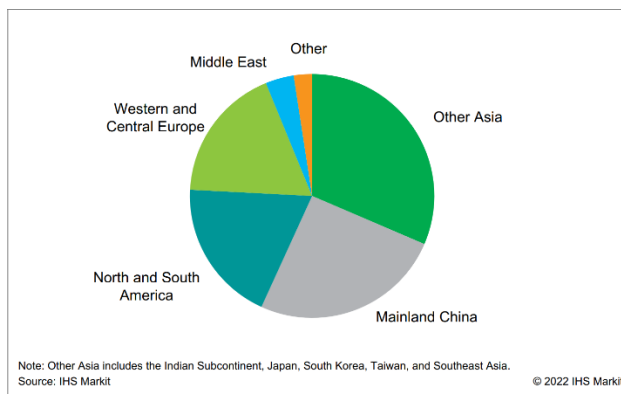


Figure 1.3.1. World consumption of cumene by 2022, retrieved from [4]

Based on Figure 1.3.1, Mainland China accounts for approximately 25% of global cumene production, equivalent to about 6.5 million metric tons per year. With a GDP of USD 19.2 trillion and a population of 1.4 billion, China provides a basis for regional scaling [7, 8]. The CIS region, with a GDP of USD 2.8 trillion and a population of 251.8 million, shows the following estimated cumene demand when scaled: about 0.948 million metric tons per year via GDP scaling and about 1.169 million metric tons per year via population scaling.

Based on that, 25% of the CIS region demand yields ~235,000 metric tons per year. However, there are certain limitations associated with the feedstock availability in the region (see

Appendix B.1); therefore, the minimum value from the range of typical capacities – 140000 tons per year for cumene production was taken as the production basis [8].

1.4 Process Selection

Among the six evaluated cumene production technologies, transalkylation was selected as the most suitable configuration based on a balanced assessment of conversion efficiency, environmental impact, and economic performance. As shown in Table 1.4.1, transalkylation achieves a propylene conversion of 99% and a reaction yield exceeding 99%, matching the best-performing conventional technology while significantly outperforming two-flash energy-integrated (97.91%) and double-effect distillation (95.97%) configurations [11]. A key advantage of this technology lies in its use of a transalkylator, which converts the undesirable by-product DIPB back into cumene, thereby increasing overall yield and reducing raw material waste [9]. This recycling of DIPB also minimizes the need for extensive downstream separation, thereby reducing operational complexity and costs, as the need for distillation columns is reduced when DIPB is continuously redirected to the transalkylator [10]. From an environmental standpoint, transalkylation produces 0.1447 MT CO₂ per MT of cumene – a notable improvement over the conventional process (0.1674 MT CO₂ per MT cumene) reported by Luyben [11], through higher than the two-flash and reactive distillation alternatives [11]. Critically, its capital expenditure of USD 5.90 million per year is substantially lower than the more energy-intensive options, such as the dividing wall column (USD 8.22 million per year) studied by Zhai et al [13] and two-flash technology (USD 7.87 million per year), making it the most economically competitive choice among the configurations that also achieve high conversion and low DIPB formation. This combination of high yield, effective by-product utilization, and favorable capital costs positions transalkylation as the optimal technology for cumene production.

Table 1.4.1. Summary of the pros and cons of different technologies

Technology	Propylene conversion, %	Reaction yield, %	DIPB formation	CO ₂ emissions, MT of CO ₂ per MT of cumene	Capital expenditure, USD million/year
Conventional	99 [12]	99 [14]	Higher than in other configurations	0.1674	5.16
Transalkylation	99 [14]	>99 [14]	Low due to the transalkylation	0.1447	5.90

Two-flash energy-integrated	97.91 [12]	>98 [14]	Low due to the energy integration	0.0365	7.87
Dividing wall column	98 [12]	99 [13]	Low due to recycling using DWC	0.0776	8.22
Reactive distillation	99 [14]	99.46 [14]	Low due to efficient control using the RD column	0.0669	5.90
Double-effect distillation	95.97 [12]	99.97	Low due to optimization of energy	0.0891	8.09

1.5 Selection of a Catalyst

For all the manufacturing options, the process is based on alkylation of benzene with propylene, but options differ in acid catalyst, conditions, and technologies, resulting in variation of advantageous and negative sides of each. There are three main manufacturing options based on the catalysts used in the alkylation process:

1. Solid-phosphoric acid (SPA) catalyst
2. Aluminum chloride (AlCl_3) catalyst
3. Zeolites-based catalyst

Zeolite-based catalysts are a modern alternative to SPA and AlCl_3 catalysts used in cumene production. Zeolites were licensed in a liquid-phase process by CDTech, Dow, Mobil-Badger, and UOP [15]. They are regenerable and environmentally friendly, meaning that zeolites can be disposed of through landfills and operated and maintained at low cost due to the absence of corrosion concerns [15].

Zeolites catalyze both the alkylation of benzene with propylene and the transalkylation of DIPB to cumene, improving efficiency [15]. The yield of produced cumene using zeolites is higher than that using other types of catalysts.

Among all zeolite-based catalysts, Zeolite- β and MCM-22 show promising results in selectivity (90.76% and 90.56%, respectively) and conversion (97.3% and 97.7%, respectively) of cumene for primary alkylation due to favorable large-pore structures and high acidity [16]. Alas, Zeolite- β has historically been a prominent option for transalkylation due to its greater stability under design conditions than other catalysts. Therefore, it is proven to be the most effective choice

in both aromatic alkylation of benzene with propene and transalkylation of diisopropylbenzene. A more detailed comparison of various catalyst types and zeolite materials is provided in Appendix B.2.

1.6 Chemical Reaction Mechanism

Zeolite-catalyzed alkylation of benzene with propylene proceeds via an electrophilic aromatic substitution mechanism. Zeolite catalysts contain Brønsted acid sites that protonate the propene double bond, generating an isopropyl carbocation. It acts as the electrophile and is attacked by the delocalized π -electrons of benzene, forming an arenium ion. Subsequent deprotonation of the ion and the proton being transferred back to the zeolite yields cumene [17].

One of the minor side reactions, the production of n-propylbenzene, occurs when a small amount of unstable primary propyl carbocation forms. It contributes to catalyst deactivation [16]. A more important side reaction is the formation of diisopropylbenzene (DIPB). This reaction takes place by a similar mechanism, in which the aromatic ring of cumene reacts with the isopropyl carbocation to form DIPB (primarily para-isomer) [18].

Cumene yield can be further improved by transalkylation of diisopropylbenzene. In this reaction, the DIPB molecule is first protonated by an acid site on the zeolite catalyst. The resulting arenium ion is then attacked by the π -electrons of a benzene molecule. The intermediate subsequently undergoes cleavage and deprotonation on the zeolite surface, producing cumene [19].

Chapter 2. Process description

2.1 PFD, Stream tables and Material Balance

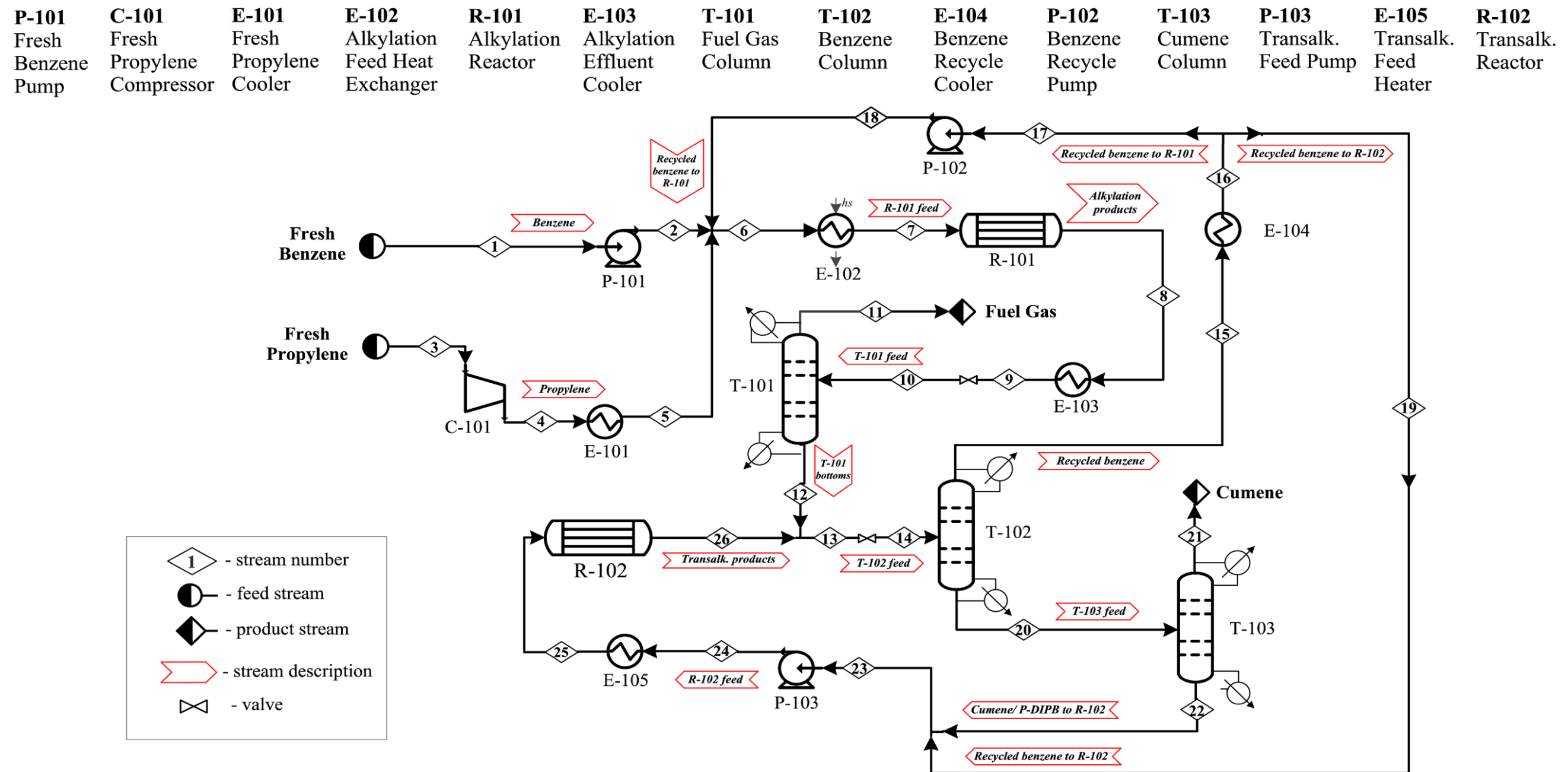
The process considered in this work is the industrial production of cumene based on the works of Pathak et al. and Nourozi et al [14], [20]. The input and output flows of the designed process are summarized in Table 2.1.1, located below. The basis for the mass balance section was set at 143 kmol/h, calculated from the plant capacity in Appendix B.1.

Table 2.1.1. Input and output streams for the designed process.

Component	M _w , kg/kmol	Input			Output		
		Stream	kmol/h	tonne/h	Stream	kmol/h	tonne/h
Benzene	78.11	Benzene feed	143.09	11.18	Fuel gas	0.1	7.2
					Cumene product	0.14	11.0

Propene	42.08	Propylene feed	147.21	6.19	Fuel gas	4.4	183.1
Propane	44.10	Propylene feed	7.39	0.33	Fuel gas	7.4	326.0
Cumene	120.19	-	-	-	Cumene product	142.86	17170.9
DIPB	162.27	-	-	-	Fuel gas	Traces	Traces
					Cumene product	Traces	Traces
Total	-	-	297.7	17696.7	-	154.9	17698.2

Process Flow Diagram



Stream number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
Temperature, °C	25	29	20	217	25	27	180	243	170	170	43	213	179	100	86	25	25	27	25	167	163	226	31	33	240	240
Pressure, bar	1.0	35.0	1.0	35.0	35.0	35.0	35.0	35.0	35.0	15.0	14.9	15.5	15.0	1.3	1.2	1.0	1.0	35.0	1.0	1.4	1.3	1.5	1.0	24.5	24.5	24.5
Vapor fraction	0.00	0.00	1.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.48	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mass flow, tonne/h	11.2	11.2	6.5	6.5	6.5	89.2	89.2	89.2	89.2	89.2	0.5	88.7	101.0	101.0	82.8	82.8	71.6	71.6	11.3	18.1	17.2	1.0	12.2	12.2	12.2	12.2
Mole flow, kmol/h	143.1	143.1	154.6	154.6	154.6	1213.6	1213.6	1070.8	1070.8	1070.8	11.8	1059.0	1209.3	1209.3	1060.4	1060.4	916.0	916.0	144.4	148.9	143.0	5.9	150.3	150.3	150.3	150.3
Component Flowrates, kmol/h																										
Benzene	143.1	143.1	0.0	0.0	0.0	1059.0	1059.0	921.4	921.4	921.4	0.1	921.3	1060.5	1060.5	1060.4	1060.4	916.0	916.0	144.4	0.1	0.1	0.0	144.4	144.4	144.4	139.2
Propylene	0.0	0.0	147.2	147.2	147.2	147.2	147.2	4.3	4.3	4.3	4.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Propane	0.0	0.0	7.4	7.4	7.4	7.4	7.4	7.4	7.4	7.4	7.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cumene	0.0	0.0	0.0	0.0	0.0	0.0	0.0	132.5	132.5	132.5	0.0	132.5	143.0	143.0	0.0	0.0	0.0	0.0	0.0	143.0	142.9	0.1	0.1	0.1	0.1	10.5
P-DIPB	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.2	5.2	5.2	0.0	5.2	5.8	5.8	0.0	0.0	0.0	0.0	0.0	5.8	0.0	5.8	5.8	5.8	5.8	0.6

Figure 2.1.1. Process flow diagram and stream table

Zeolites are commonly used in liquid-phase cumene production processes (for both alkylation and transalkylation reactions), according to CDTech, Dow, and Mobil-Bagder [15]. The operating conditions of the first reactor R-101 were taken from the work of Corma et.al., which concluded that a temperature of 180°C and a pressure of 35.0 bar are optimal parameters for the highest selectivity of cumene – 91.59% (by propylene) and conversion of propylene – 97.34% [16] (calculations are given in Appendix B.3.). The reaction in alkylator takes place in excess of benzene, with a favorable benzene to propylene ratio (B/P ratio) of 7.2 [16]. Meanwhile, the operating conditions for the transalkylator R-102 were set to 240°C, 24.52 bar, and a benzene-to-DIPB (B/DIPB) ratio of 25 (see Appendix B.3. for conversion of pressure units) [21]. Under these conditions, the conversion of DIPB was set as 90% [5].

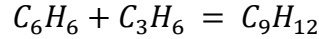
The operating conditions and separation efficiencies for distillation columns were taken from the work of Norouzi et al., in which the cumene production process also occurs in a liquid phase using zeolite-based catalysts [20]. The first distillation column, T-101, operates at 170°C and 15 bar, with nearly 100% separation of propylene and propane from reactor effluent. The second and third distillation columns, T-102 and T-103, operate at 1.3 bar and 1.4 bar, respectively. T-102 benzene column operates at 99.6°C, while T-103 cumene separation column operates at 96°C. The columns have the following separation efficiencies: 99.99% of benzene and nearly all cumene go to the top product; 100% of DIPB goes to the bottom product; the third column separates cumene into the distillate with 99.99% efficiency, and 99.98% of DIPB goes to the bottom product. To maintain specified B/P and B/DIPB ratios, split fractions for the benzene recycle stream, as well as flow rates of feed streams, were calculated using the Design Specification tool in Aspen Plus (see ESI), which resulted in 0.1362 and 0.8638 for the transalkylator benzene feed and alkylator recycle feed.

In the chosen transalkylation technology demonstrated in Figure 3, fresh benzene enters the system at standard conditions (25°C and 1 bar) with a flow rate of 143.1 kmol/hr, and propylene (95 wt% propylene and 5 wt% n-propane) stream enters the system at 20°C and 1 bar with a flow rate of 154.6 kmol/hr. C-101 then compresses the propylene feed stream to a liquid state at 217 °C and 35 bar, and is cooled by cooler E-101 to 25 °C, while the benzene feed goes through P-101 pump to reach 35 bar. Feed streams are then mixed with the recycled benzene stream with a flow rate of 916.0 kmol/hr, which was pumped (P-102) to an operating pressure of R-101 (35.0 bar). The resulting mixture at 1213.6 kmol/hr is then heated to 180°C in a heat exchanger (E-102) and fed to the alkylation reactor (R-101). The reaction takes place at 180°C and 35.0 bar and in the liquid phase. The reactor effluent is cooled down in the cooler (E-103) to 170 °C. Following that, the pressure of the cooled product decreases in the valve to 15 bar and is sent to the first distillation column (T-101), where propylene and propane are separated. All the propane and propylene are removed as fuel gas (top product) at 4.3 kmol/hr and 7.4 kmol/hr, respectively. The bottoms of the first column, which are benzene at 921.3 kmol/hr, cumene at 132.5 kmol/hr, and DIPB at 5.2 kmol/hr, are mixed with effluent from the transalkylator consisting of benzene, cumene, and DIPB at 139.2 kmol/hr, 10.5 kmol/hr, and 0.6 kmol/hr, respectively. The mixed stream pressure is first

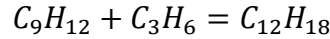
reduced to the operating pressure of the second distillation column (1.3 bar) and then sent to the second distillation column (T-102), where isobenzene is separated from cumene and DIPB. In the second distillation column, benzene is recovered as distillate. The bottom product from the column is fed to the third column (T-103), where 99.9 mol% of cumene is recovered as the top product. DIPB is collected at a flow rate of 5.8 kmol/hr as the bottom product and then sent to the transalkylation unit (R-102), where the reaction occurs in the liquid phase. The bottom product of the third column is mixed with a fraction of recycled benzene (144.4 kmol/hr), pumped (P-103) to 24.5 bar, heated (E-105) to 240°C, and fed to the transalkylation reactor. The top of the third column is collected at a flow rate of 143 kmol/hr, which consists of 99.9% cumene.

2.2 Kinetics

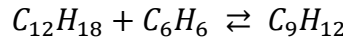
The kinetics of both alkylation and transalkylation reactions are described using a simplified Eley-Rideal to Power Law model. The reaction rate equations are given as follows [20]:



$$r_1 = 6510 \exp\left(-\frac{52564}{RT}\right) C_P \quad (1)$$



$$r_2 = 450 \exp\left(-\frac{55000}{RT}\right) C_P \quad (2)$$



$$r_f = 2.529 \times 10^8 \exp\left(-\frac{100000}{RT}\right) x_B x_D \quad (3)$$

$$r_b = 3.877 \times 10^9 \exp\left(-\frac{127240}{RT}\right) x_C^2 \quad (4)$$

In Equations 1 and 2, r_1 and r_2 denote the reaction rates for the formation of cumene and DIPB via alkylation (kmol/m³ s), respectively, with C_P representing the propene concentration (kmol/m³). In Equations 3 and 4, r_f and r_b describe the forward and reverse transalkylation rates (kmol/m³ s), while x_B , x_D , and x_C denote the molar fractions of benzene, DIPB, and cumene.

Chapter 3. Design of Major Units

3.1 Design of Heat Exchanger E-102

Overview

A heat exchanger is an industrial piece of equipment that allows heat transfer between two or more fluids at different temperatures without mixing. The heat exchanger enables the transfer of energy from a hotter fluid to a cooler one, which is substantial because no cross-contamination occurs. All such equipment, regardless of design, follows the fundamental laws of Thermodynamics. Firstly, the 1st Law of thermodynamics states that energy cannot be created or destroyed; it can only be converted from one form to another, meaning that the total heat energy of the two process streams in a closed system is the same before and after the heat exchanger. Secondly, the heat always moves from hot to cold objects. This is because heat cannot spontaneously move from a colder to a hotter object thermodynamically [22].

Heat Exchanger Type Selection

Heat exchanger selection is based on fluid properties, required heat duty, and process objectives (heating, cooling, or heat recovery). Space limitations and pressure drop constraints must also be considered. Moreover, capital costs, operating expenses, and maintenance expenses are essential to ensure reliable and economically efficient performance [23]. Based on the requirements above, a shell-and-tube heat exchanger is chosen as it is the most widely known, versatile, and operates over a wide range of temperatures and pressures. Despite its advantages, this type of heat exchanger has lower thermal efficiency than other types and contains stagnant zones on the shell, which can lead to corrosion [24].

Table 3.1.1. Heat exchanger type selection

Feature	Selection	Justification
Front head	B (bonnet)	Standard pressure-tight construction
Shell type	E (single-pass)	Appropriate for condensing duty
Rear head	M (Fixed tubesheet)	Strong construction, lower cost
Tube layout	Triangular pitch	Better heat transfer

Working Principle of the Unit

The E-102 is designed to heat mostly benzene and propylene to reactor operation temperature. It also plays a substantial role in the design process, as the main reaction (alkylation) requires heat to proceed. Therefore, it is required to heat 1216.5 kmol/hr of inlet mixture from 27.4 °C to 180 °C for further processing in the reactor. The heat exchanger's heat duty is 7469 kW. To design the heat exchanger, the following steps were considered:

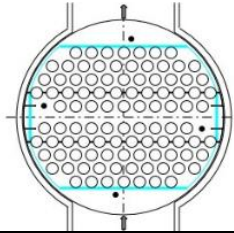
1. Defining the known operating parameters, including inlet and outlet temperatures and the mass (or molar) flow rate of the process stream.
2. Determining the required heat duty based on the flow rate and enthalpy change of the process fluid.
3. Choosing an appropriate exchanger configuration based on process conditions and mechanical considerations.
4. Assuming a reasonable overall heat transfer coefficient based on the physical properties and nature of both the process and service fluids.
5. Estimating tube length, tube diameter, and required heat transfer area.
6. Obtaining relevant thermophysical properties of both fluids: viscosity, thermal conductivity, density, and heat capacity.
7. Calculating the actual overall heat transfer coefficient and comparing it with the initially assumed value.
8. Determining pressure drops on both shell and tube sides and verifying the compliance with Aspen results.
9. Revising the geometrical assumptions again until convergence, if the calculated parameters do not satisfy thermal or hydraulic requirements.

Table 3.1.2. Inlet and outlet stream values.

Parameter	Unit	Shell side (mixture of fluids)	Tube side (condensed steam)
T inlet	°C	27.4	242.6
T outlet	°C	180	242.2
Flow rate	kmol/hr	1216.5	821.3
Flow rate	kg/hr	89460.5	14795.7
P inlet	bar	35	35

P outlet	bar	34.7	35.0
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Table 3.1.3. Heat exchanger design

E-102 heat exchanger specification sheet		
		
Parameter	Tube side	Shell side
Length, m	4.9	
Inner diameter, mm	17.3	447
Outer diameter, mm	19	465
Tube pitch/baffle spacing, mm	23.75	178
Arrangement	30° triangular	Horizontal, single segmental
Tube/shell passes	1	1
Number of tubes (tubes per pass)/baffles	215	26
Pressure drop, kPa (calculated)	43.1	2.8
Material	Carbon steel	

Estimated area, m ²	52.5
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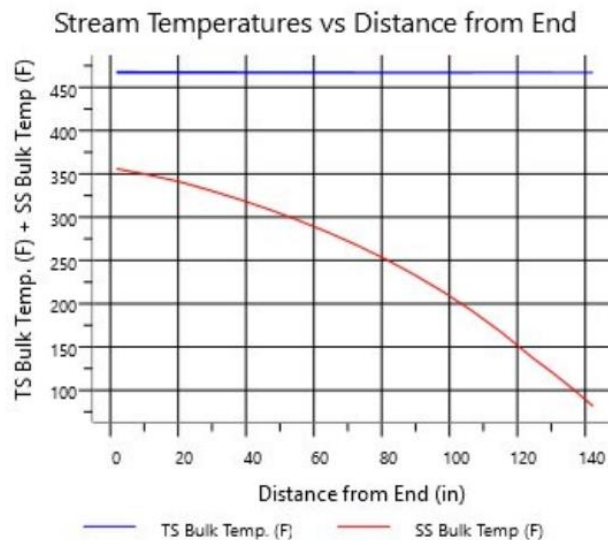


Figure 3.1.1. Graph of the temperatures for both sides

The constant temperature on the tube side indicates that condensation is occurring effectively, resulting in relatively low thermal resistance during heat transfer. Even though significant fouling is present and the relatively low thermal conductivity of carbon steel is considered, the overall heat transfer performance remains satisfactory.

The following table compares EXCEL's calculation results with Aspen's results. It can be observed that the deviation between Excel results and validated values is insignificant. Possible reasons for these deviations are:

1. Different property models: Aspen uses rigorous thermodynamics while Excel often uses constant or averaged values.
2. Temperature-dependent properties: Aspen updates along the exchanger length, whereas Excel might not.
3. Different heat transfer correlations: HTRI/TEMA in Aspen and simplified formulas in Excel.
4. Iteration and rounding differences.

Table 3.1.4. Excel vs. Aspen results

Parameter	Excel Calculation	Aspen (HeatX/EDR)
-----------	-------------------	-------------------

Heat duty, kW	7469.38	7469.94
LMTD, °C	118.494	118.003
Overall U_{clean} , $\text{W}\cdot\text{m}^2\cdot\text{K}$	2060.75	1999.32
Shell-side film coefficient, $\text{W}\cdot\text{m}^2\cdot\text{K}$	2731.09	2742.49
Tube-side film coefficient, $\text{W}\cdot\text{m}^2\cdot\text{K}$	11058.1	11851.6
Required Area, m^2	52.75	52.4585
Tube-side pressure drop, kPa	2.84	3.06
Shell-side pressure drop, kPa	43.09	45.00

3.2 Design of Reactors R-101 and R-102

Overview

In cumene production over zeolite catalysts, an adiabatic multitubular fixed-bed reactor is utilized. In this design, solid beta-zeolite particles are packed inside parallel tubes, while liquid reactants flow through the catalyst bed. This configuration is widely used in heterogeneous catalytic processes, as it provides high conversion efficiency, enables effective temperature management, and therefore reduces the risk of catalyst deactivation [25].

Due to the exothermic nature of the alkylation reaction, the reactors operate under adiabatic conditions, resulting in a slight temperature increase along the catalyst bed. To prevent excessive temperature rise, coolers are installed after both reactors.

Material Selection

ASTM A106 Grade B was selected for the reactors due to its good mechanical strength and reliability at elevated temperatures and pressures, maintaining adequate strength and structural integrity under such conditions. It also provides sufficient thermal conductivity, allowing for the minimization of temperature gradients and hot spots within the reactor. In addition, its availability and relatively low cost make it more practical than other materials [26].

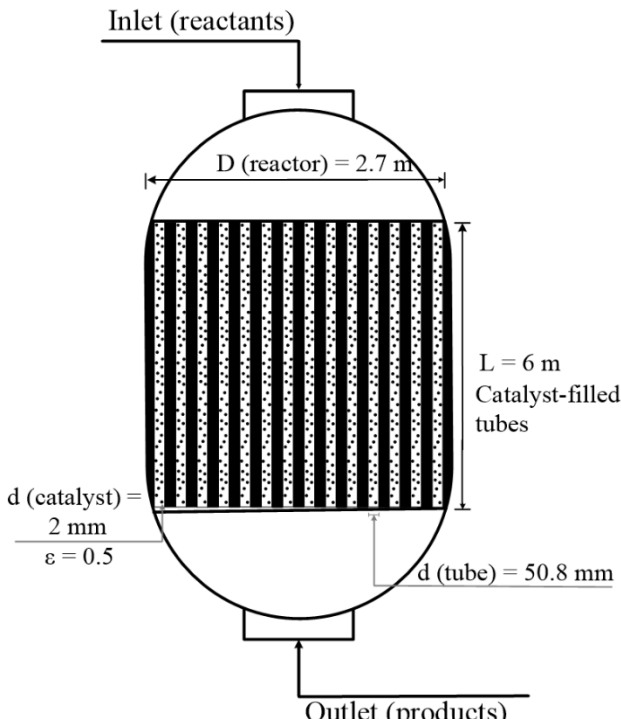
Reactor Tube Dimensions

The reactor tube configuration was adjusted to meet manufacturing standards, enabling better conversion and reduced pressure drop. Thus, the following parameters were selected: $L = 6$ m, $d_{in} = 50.8$ mm (2 in). The outer diameter of the tube was chosen in accordance with the nominal standard orders listed in ASME B36.10, which is 60.33 mm (2.375 in). Wall thicknesses, therefore, were calculated to be 2.72 mm (R-101) and 2.43 mm (R-102), considering the corrosion allowance and Mill tolerance (12.5%) to ensure that the tube does not break or deform under pressure. The number of tubes was calculated by using the design specification of 97% and 90% conversion for R-101 and R-102, respectively.

Assumptions made for the adiabatic fixed reactor:

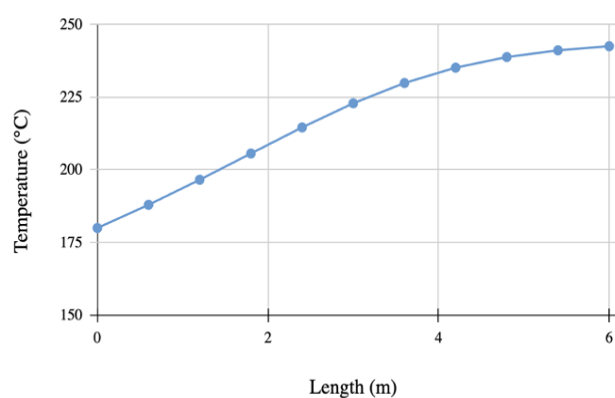
- The process operates under steady-state conditions for variables such as temperature, pressure, and molar flow rates.
- Only the liquid phase is present in the reactor; hence, vapor-liquid equilibrium and vaporization enthalpy are not accounted for in the phase change; only the slightly exothermic reaction energy is considered, resulting in a small temperature increase.
- In fixed-bed reactors, the catalyst particle size ranges from 2 to 5 mm [27].
- Design pressure is 10% higher than the operating pressure to account for catalyst deactivation or changes in feed composition.
- Design temperature includes a safety margin of +25°C above the highest expected temperature along the reactor length to ensure a suitable material selection and reduce the probability of plastic deformation.
- When irregularly shaped zeolite particles are used in fixed-bed reactors, the bed porosity is in the range between 0.48 and 0.51 [28].
- It is assumed that the catalytic zeolite particles are perfectly spherical.
- Near-ideal plug-flow behavior in each tube is assumed, with no axial mixing and minimal hot-spot formation.

Table 3.2.1. Design specifications for R-101 and R-102

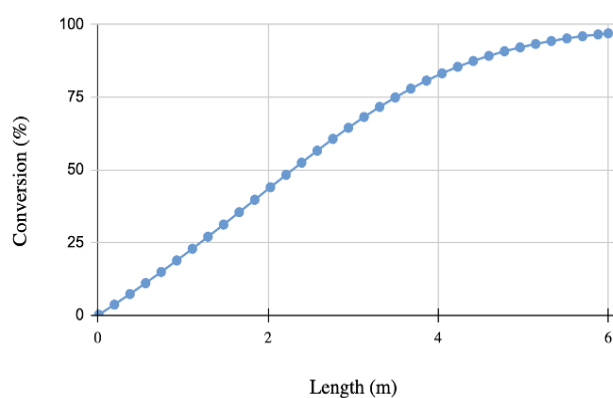
DATA SHEET FOR R-101 and R-102		
Operating and Mechanical data		
 Inlet (reactants) $D \text{ (reactor)} = 2.7 \text{ m}$ $L = 6 \text{ m}$ Catalyst-filled tubes $d \text{ (catalyst)} = 2 \text{ mm}$ $\varepsilon = 0.5$ $d \text{ (tube)} = 50.8 \text{ mm}$ Outlet (products)		
	R-101	R-102
Reactor type	Adiabatic fixed bed reactor	
Operating pressure, bar	35.0	24.5
Design pressure, bar	38.5	26.95
Inlet temperature, °C	180.0	240.0
Design temperature, °C	267.5	288.4

Outlet temperature, °C	242.5	240.05
Number of tubes	1223	1010
Length, m	6	
Inner diameter, mm	50.8	
Outer diameter, mm	60.33	
Volume of the reactor, m ³	14.92	12.28
Volume of a parallel tube, m ³	0.012	
Wall thickness, mm	2.72	2.43
Bed voidage	0.5	
Material	Carbon steel	
Construction code	ASTM A106 Grade B	
Minimum yield strength, kpsi	35.0	
Minimum tensile strength, kpsi	60.0	
Allowable stress (S), kpsi	17.3	
Corrosion allowance, mm	1.5	
Quality factor (E)	1	
Coefficient (Y)	0.4	

Process data		
	R-101	R-102
Catalyst loading, kg	3730	3070
Superficial velocity, m/s	0.016	0.0042
Actual velocity, m/s	0.032	0.053
Pressure drop, bar	0.041	0.0055
Catalyst data		
Catalyst type	Beta zeolite	
Catalyst density, kg/m ³	1000	
Particle size diameter, mm	2	
Shape factor	1	



(a)



(b)

Figure 3.2.1. a) Temperature vs. Reactor length graph for R-101 and b) Conversion of propene vs. Reactor length graph for R-101

Figure 3.2.1(a) illustrates the temperature profile along with the reactor length. As the reacting mixture flows through the reactor, the temperature gradually increases from 180°C to 242.5°C. The overall temperature rise indicates the exothermic nature of the alkylation reaction. It is also observed that the temperature increase is rapid in the initial section of the reactor, but it slows down further along the length. It indicates that the reaction rate decreases as the limiting reactant is progressively consumed.

Figure 3.2.1(b) shows the variation of propene conversion with reactor length, which was obtained through sensitivity analysis of the alkylator. The resulting data shows that conversion approaches nearly 100% at a reactor length of 6 meters. Extending the reactor length beyond this value is not economically justified, as it increases capital costs and pressure drop. Therefore, this choice was made between achieving higher conversion and minimizing equipment design costs.

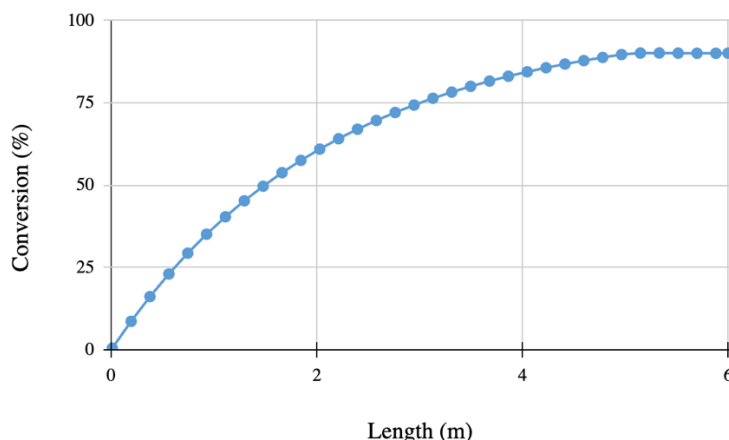


Figure 3.2.2. Conversion of DIPB vs. Reactor length graph for R-102

Figure 3.2.2 illustrates how conversion changes along the reactor length. The target conversion of 90% is achieved at approximately 5 m. However, to account for potential vapor-phase formation at elevated temperatures and to maintain consistency in the design of both alkylation and transalkylation reactors, a length of 6 m was selected.

3.3 Design of Distillation Columns T-101, T-102, and T-103

Overview

This section outlines the general design of the methodology, governing equations, and the heuristic assumptions applied in the preliminary design of the distillation columns – T-101, T-102, and T-103. The common rules and shortcut calculations were applied uniformly across all three columns to establish a consistent design basis that remains relevant to the available literature. A more detailed description of each column, including its specific operating conditions and optimized design parameters, is provided in the subsequent sections.

The following common heuristics and general parameters were used:

1. Tray spacing is usually 0.5-0.6 m for accessibility. All 3 distillation columns (T-101, T-102, T-103) have a tray spacing of 0.6096 m, which is automatically suggested by Aspen Plus.
2. All sieve holes have a diameter of 6-7 mm.
3. The economically optimal reflux ratio is in the range of 1.2 to 1.5 times R_{min} .
4. The Fenske-Underwood-Gilliland (FUG) shortcut method is used to estimate the minimum number of trays, the theoretical number of trays, and the minimum and actual reflux ratios.

Type of Trays

For all three distillation columns, sieve trays were selected based on performance and economic considerations. Compared to bubble-cap trays, sieve trays are more advantageous in terms of efficiency, capacity, construction, and capital cost. Based on experimental studies, it was concluded that properly designed sieve trays maintain high, nearly constant tray efficiency, whereas bubble-cap trays fluctuate in efficiency and exhibit higher entrainment at elevated loads [29]. In addition, the structure of sieve plates is simpler than that of bubble-cup trays, resulting in lower manufacturing costs and easier installation [29].

Material Selection

SA-516 Gr. 70 carbon steel (ASME SA-516 Grade 70) was selected for the three distillation columns because it is widely used in pressure-containing equipment such as pressure vessels, boilers, and petroleum tanks [30]. This material provides adequate mechanical strength, with a nominal tensile strength of 485-620 MPa and a minimum yield strength of 260 MPa [30]. Moreover, the plates were tested, and it was concluded that they exhibited a yield strength of up to 385 MPa. Consequently, SA-516 Gr. 70 carbon steel is appropriate for withstanding operating pressures in distillation columns, such as 15.5 bar in T-101, 1.419 bar in T-102, and 1.543 bar in T-103.

Main Calculations

The following equations are applied for the calculations of key design and operating parameters of the distillation columns:

- Antoine's equation to estimate saturation pressure (C_{1i-7i} parameters are summarized in Table C.3.1) retrieved from Aspen Plus v14:

$$\ln p_i^{sat} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{6i}T^{C_{7i}} \quad (5)$$

where p^{sat} is saturation pressure (bar), C_{1i-7i} are Antoine equation parameters, and T is temperature (K).

- K-value approximation from Raoult's law [31]:

$$K_i = \frac{y_i}{x_i} = \frac{p_i^{\text{sat}}}{p_i}, \quad (6)$$

where K_i is the K-value, y_i is the vapor molar fraction, x_i is the liquid molar fraction, and p_i is the pressure (bar).

- Relative volatility, α [32]:

$$\alpha_{ij} = \frac{K_i}{K_j} \quad (7)$$

$$\alpha_{ij} = \sqrt{\alpha_{\text{top}} \alpha_{\text{bottom}}} \quad (8)$$

- Fenske equation to estimate the minimum number of stages [32]:

$$N_{\min} = \frac{\log \left[(x_i/x_j)_D / (x_i/x_j)_B \right]}{\log \alpha_{ij}}, \quad (9)$$

where D and B indices mean distillate and bottom, respectively; x_i is the molar fraction of LK component, x_j is the molar fraction of HK component, and α_{ij} is the relative volatility of LK to HK components.

- Underwood to estimate the minimum reflux ratio [8]:

$$\sum \frac{\alpha_i x_{i,f}}{\alpha_i - \theta} = 1 - q, \quad (10)$$

$$\sum \frac{\alpha_i x_{i,d}}{\alpha_i - \theta} = R_{\min} + 1, \quad (11)$$

In which α_i is the relative volatility of component I to HK component, $x_{i,f}$ is the molar fraction of component i in the feed, θ is the root of the equation, and q is the feed enthalpy condition parameter. The value of θ must be in the range between 1 and the relative volatility of LK to HK.

- Feed enthalpy condition parameter [32]:

$$q = \frac{H_V - H_F}{H_V - H_L} \quad (12)$$

where H_V is the molar enthalpy of vapor (kJ/mol), H_F is the molar enthalpy of feed (kJ/mol), and H_L is the molar enthalpy of liquid (kJ/mol).

- Gilliland for the theoretical number of stages optimization [32]:

$$\frac{N - N_{min}}{N + 1} = 1 - \exp\left(\frac{1 + 54.4\psi_G}{11 + 117.2\psi_G} \times \frac{\psi_G + 1}{\psi_G^{0.5}}\right), \quad (13)$$

$$\psi_G = \frac{R - R_{min}}{R + 1}, \quad (14)$$

in which N is the number of theoretical stages, N_{min} is the minimum number of stages, ψ_G is the Gilliland correlation coefficient, R is the reflux ratio, and R_{min} is the minimum reflux ratio.

The Aspen Plus simulation was initialized from the DSTWU column model design, which uses the FUG shortcut method to estimate the minimum and actual reflux ratios and the minimum and theoretical numbers of stages. This preliminary design was mainly used to check hand calculations. Subsequently, the RadFrac model was developed to enable more detailed design and internal optimization. Unlike the shortcut method, the RadFrac model performs detailed stage-by-stage calculations, accounts for property variations throughout the column, and enables the specification and design of internal column parameters.

One of the most important specifications of the column is the Murphree efficiency parameter, which measures the effectiveness of an individual tray in the distillation column. It is defined as the ratio of the actual compositional change to the ideal change under equilibrium conditions [32]. To estimate the value of Murphree efficiency, the following empirical correlation was used [32]:

$$E_a = \frac{E_{mV}}{1 + E_{mV} \left[\frac{\psi}{1 - \psi} \right]} \quad (15)$$

In Equation 15, E_{mV} is the Murphree efficiency, E_a is the actual column efficiency, and Ψ is the fractional entrainment. To use this correlation, actual column efficiency was assumed to be equal to the efficiency estimated by O’Connell’s correlation [32]:

$$E_0 = 51 - 32.5 \log(\mu_a \alpha_a), \quad (16)$$

where μ_a is the molar average liquid viscosity (mNs/m^2), α_a is the average relative volatility of the light key. Average viscosity was estimated as the geometric mean at the top and bottom streams of the column.

Entrainment estimation is detailed in Appendix C.3, where it is determined from correlations among the percentage flooding, flooding vapor velocity, and liquid-vapor flow factor.

To estimate diameter, the following formula was used [32]:

$$D_c = \sqrt{\frac{4\hat{V}_w}{\pi \rho_v \hat{u}_v}}, \quad (17)$$

where $\hat{V}_w$ is the maximum vapor rate (kg/s), ρ_v is the maximum vapor density (kg/m^3), and $\hat{u}_v$ is the maximum allowable vapor velocity (m/s), which is estimated by the following equation:

$$\hat{u}_v = (-0.171l_t + 0.27l_t - 0.047) \left[\frac{\rho_L - \rho_v}{\rho_v} \right]^{1/2} \quad (18)$$

In Equation 18, l_t is the tray spacing (m), ρ_L is the average liquid density, and ρ_v is the maximum vapor density.

Length was estimated via the following expression [32]:

$$L = 1.2 \times l_t \times (N - 2) \quad (19)$$

Thickness is calculated by:

$$t = \frac{P_i D_i}{2SE - 1.2P_i}, \quad (20)$$

in which P is the maximum pressure (bar), D is the column diameter (m), S is the maximum allowable stress (M/mm²), and E is the weld joint efficiency.

3.3.1 Depropanizer T-101

Overview

The T-101 distillation column separates the unreacted propene and inert propane from the heavier part of the reactor R-101 effluent - benzene, cumene, and DIPB. Overall, the column prevents contamination of the product stream (cumene) and further conversion of cumene into DIPB in the transalkylator reactor. The distillate product (C3 hydrocarbons) of the column is collected in the form of vapor, while heavier components undergo further separation steps.

The separation mechanism relies on the difference in relative volatility between the light-key (LK) and heavy-key (HK) components. Propane was chosen as the light key because propene has a lower boiling point (-47.7 °C) than propene (-42.11 °C), making propene more volatile and easier to go overhead. Therefore, propane is less volatile than the heaviest component in the distillate. Benzene was chosen as the heavy key because it is the lightest component in the bottoms, owing to a much lower boiling point (80.09 °C) than that of cumene (152.41 °C) and p-DIPB (210.5 °C). Thus, benzene is the most volatile component that must remain in the bottoms and define the separation boundary. When heat is supplied in the reboiler, propane and propene vaporize and rise through the sieve trays, while benzene, cumene, and DIPB remain primarily in the liquid phase and flow downward. Counter-current contact between rising vapor and descending liquid enables mass transfer and progressive enrichment of light components toward the top of the column. The overhead vapor is condensed and partially returned as reflux to improve separation efficiency, while the heavier aromatic mixture is withdrawn as the stabilized bottoms product. The partial vapor condenser was used because distillate is removed as vapor [33].

Type of Design and Operating Conditions for the T-101 Column

The operating conditions were retrieved from the conventional transalkylation process of Pathak et al., with an inlet stream pressure of 15 bar and a temperature of 170°C [14]. The column pressure drop is 0.65 bar (difference between top and bottom), which is within the typical range for distillation columns of 5-10 psia.

Design and Calculations for the T-101 Column

The separation was defined based on propane and benzene as the primary function of the first distillation column to separate fuel gas (propane and propene) from the heavier aromatic components (benzene, cumene, p-DIPB). The propane recovery in distillate was specified at 0.999 to ensure efficient removal of the fuel gas stream, while benzene recovery was set to 0.0001 to prevent aromatics loss to the overhead. The specification was applied to calculations and the Aspen DSTWU simulation.

Hand calculations were performed to support the design. Firstly, K values for each component in the distillate and bottoms were calculated using Raoult's law, where saturation pressures were obtained from Aspen Plus v14 at the corresponding temperature and pressure conditions of the distillate and bottoms. The Antoine equation was not used because operating temperatures of propane and propene exceed their critical temperatures, at which a distinct liquid-vapor equilibrium no longer exists, and Antoine correlations are invalid. In these cases, saturation pressures were obtained from Aspen, which can handle supercritical conditions. The geometric mean K value of the top and bottom of the same component was calculated and used in relative volatility calculations in Equations 6-8.

Finally, calculations based on FUG equations were performed to find N_{min} , R_{min} , and R using Equations 5-14, respectively. The hand-calculated number of stages (N), 16, was used as input to DSTWU, and results were obtained. Calculated values of N_{min} , R_{min} , and R were compared with the Aspen Plus V14 DSTWU column simulation. Results are summarized in Table 3.3.1.:

Table 3.3.1. Hand-calculated values and DSTWU results summary

Parameter	FUG calculations	DSTWU results	Relative error, %
N_{min}	5.120	6.740	24.084
R_{min}	0.181	0.417	56.520
R ($R = 1.2 * R_{min}$)	0.217	0.508	57.209

The hand-calculated values of N_{min} , R_{min} , and R are different from those from Aspen Plus DSTWU results because the system has non-ideal behavior shown in Appendix C.3. In the hand calculations that were performed using the FUG equations, which assume ideal vapor-liquid equilibrium and Raoult's law without accounting for activity coefficient, caused the difference in results. Aspen Plus V14 software incorporates thermodynamic models that account for activity coefficients and non-ideal phase interactions.

Then, the RadFrac unit was optimized to achieve the required component recoveries by performing several sensitivity analyses on the number of stages, reflux ratio, and feed stage location, as shown in the corresponding figures. It was necessary to determine the optimal values of these parameters so that benzene recovery in the bottoms was at least 99.99% and propane

recovery in the distillate was at least 99.9%, while maintaining reasonable energy consumption and column dimensions.

Table 3.3.2. Effect of total stage number on reflux ratio and energy duties for column T-101.

N_{stages}	16	17	18	19
N_{feed}	5	5	5	6
Q_C , kW	-622.019	-485.620	-419.873	-394.609
Q_R , kW	3183.312	3046.906	2981.166	2955.894
R	9.437	7.322	6.349	5.940

According to the sensitivity analysis results, increasing the number of stages from 16 to 19 reduces the reflux ratio and both condenser and reboiler duties, improving energy efficiency. However, since column height and capital cost increase with additional trays, the optimal point is where further savings become minor. As shown in Table 3.3.2, moving from stage 18 to 19 only slightly decreases the reflux ratio and condenser and reboiler duties, while the column height increases. Therefore, 18 stages were selected as the optimal number and are within an allowable 10% safety margin, which is applied as a safety consideration based on heuristics.

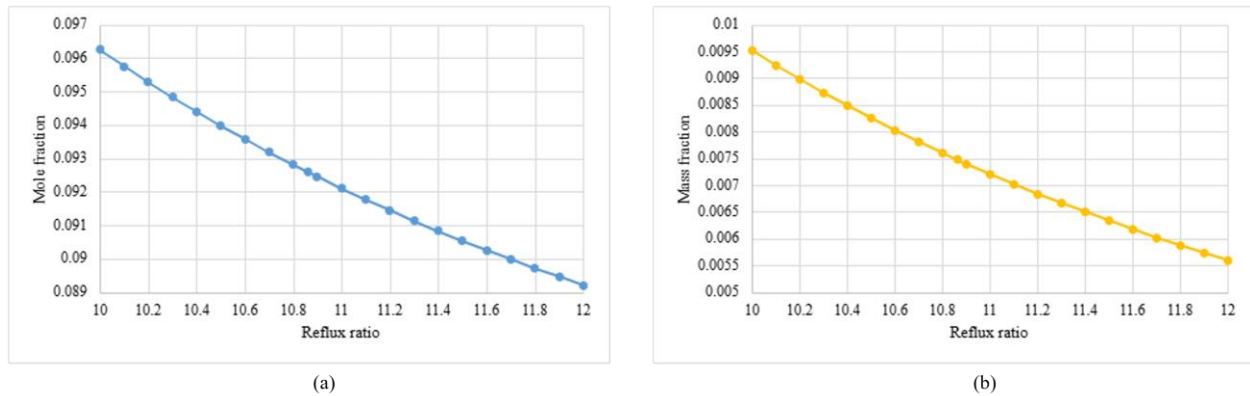


Figure 3.3.1. Benzene mass fraction in distillate (a) and propane mass fraction in bottom (b) vs reflux ratio

Figures 3.3.1 (a) and 3.3.1 (b) show the effect of reflux ratio on the benzene mole fraction in the distillate and the propane mass fraction in the bottoms, respectively. From Figure 3.3.1 and Appendix C.3, the design specifications required the mass fraction of propane in the bottoms stream to be equal to or lower than 0.0075, while the mole fraction of benzene in the distillation stream had to be equal to or lower than 0.0926. As the reflux ratio increases, both impurity levels decrease, and it can be seen that in the reflux ratio range of 10.8 to 10.9 both separation requirements are satisfied. Within this acceptable range, a reflux ratio of 10.863 was selected using

the Design Spec tool. This value was chosen to provide stable compliance with the required purities, while keeping the benzene content in the distillate as low as possible and maintaining a high propane concentration in the distillate stream, which is important for fuel gas purity. At the same time, this reflux ratio helps avoid unnecessarily high condenser and reboiler duties, thereby reducing energy consumption and operating costs.

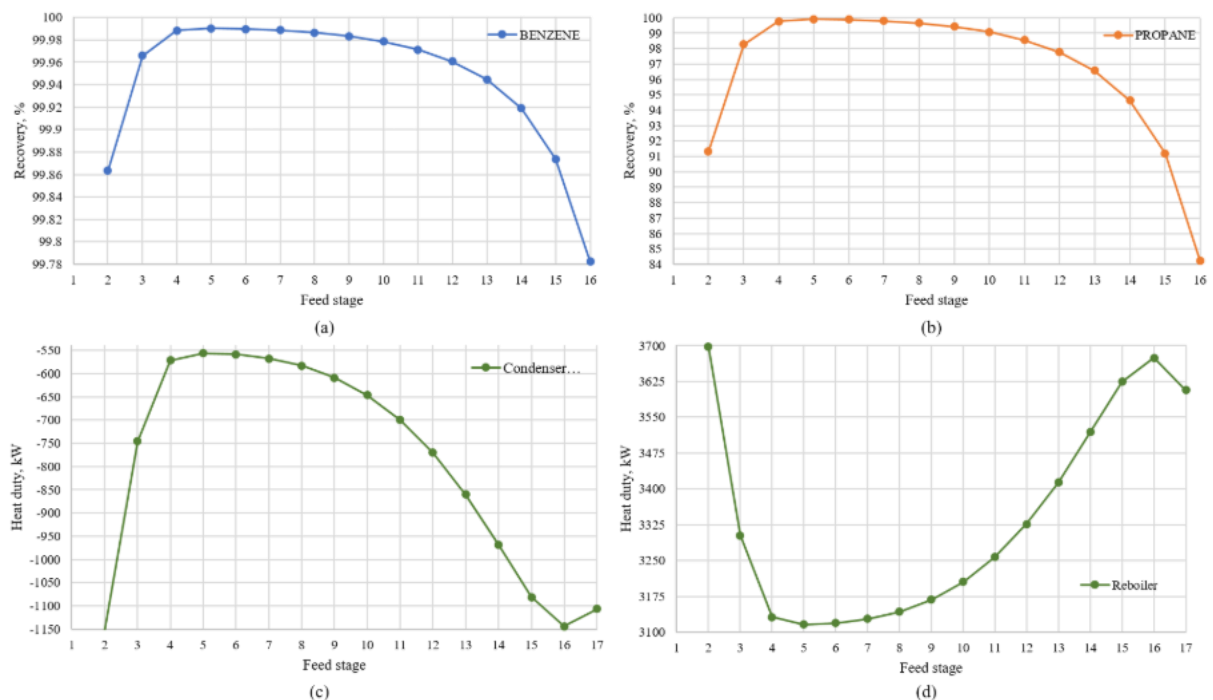


Figure 3.3.2. Feed stage optimization via the evaluation of a) recovery of benzene, %, b) recovery of propane, % c) condenser duty, kW and d) reboiler duty, kW

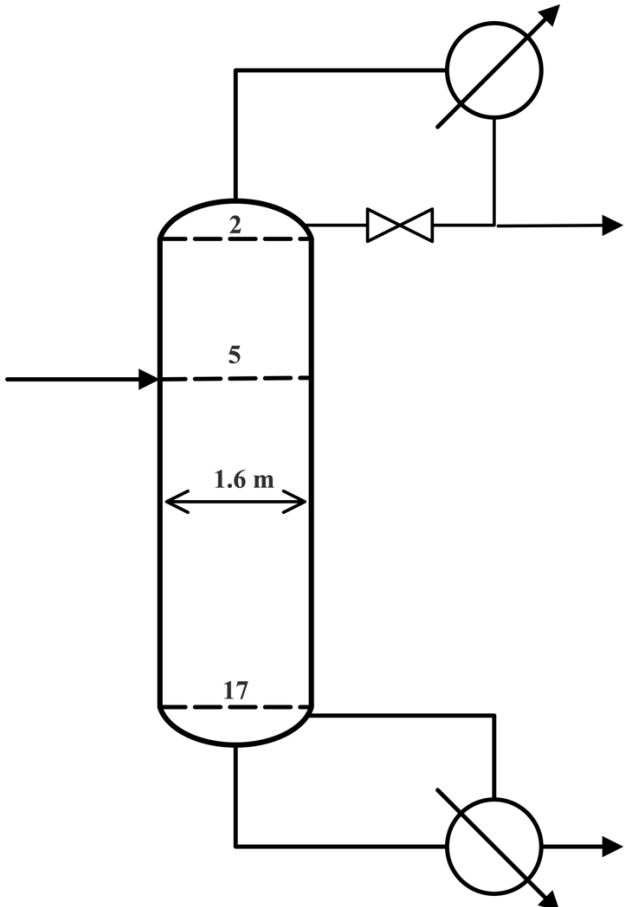
From Figure 3.3.2 (a, b), it was shown that the recovery requirements are satisfied and equal to 99.9% of benzene recovery in the bottoms and 99.902% of propane recovery in the distillate when the feed is introduced at stage 5, which corresponds to the results from Figure 3.3.2 (c, d). At stage 5, the condenser and reboiler duties were compared, identifying the most energy-efficient configuration as the reboiler duty reaches its minimum, which is equal to 3116.326, and the condenser duty is also the lowest value, equal to -556.059. Therefore, the feed stage was selected as 5, providing the required recoveries and minimizing energy consumption.

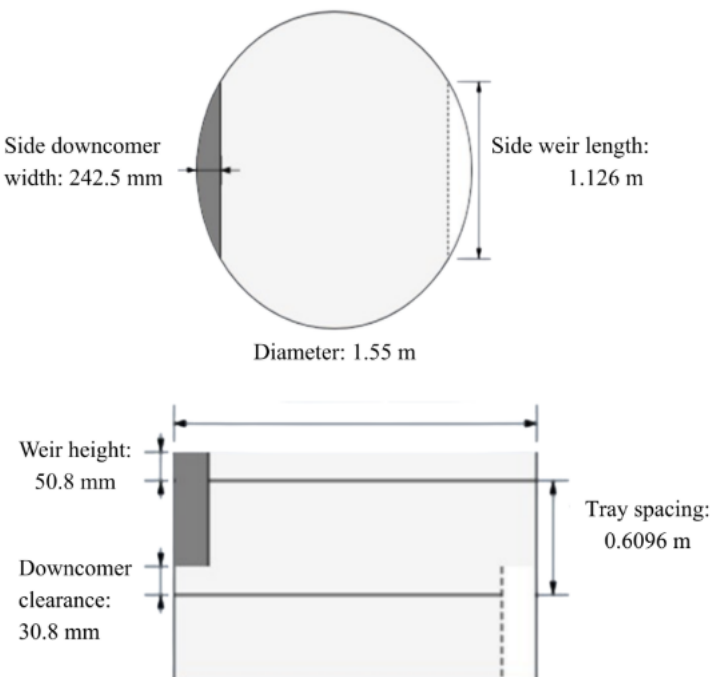
T-101 Internals Design

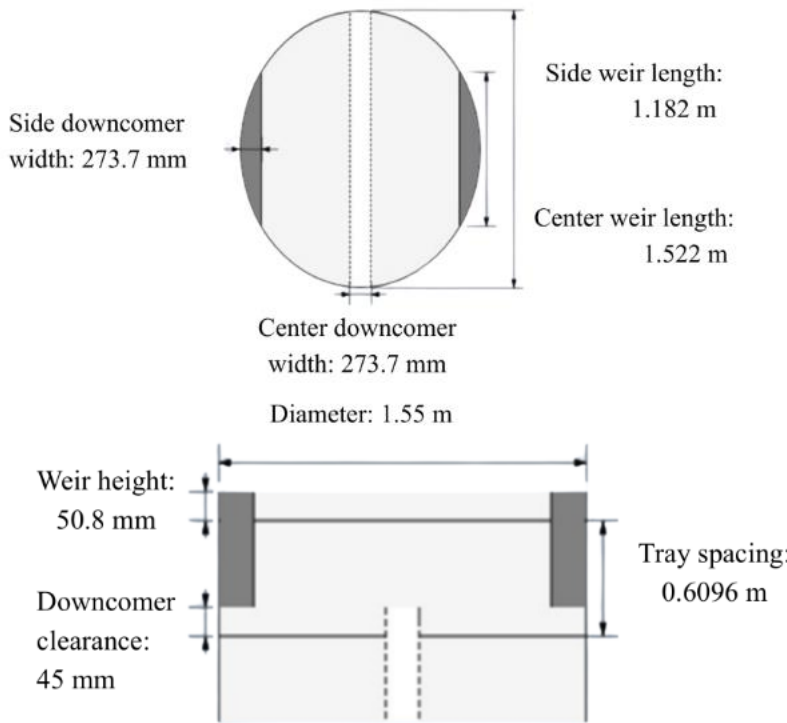
Murphree plate efficiency was calculated using Equations 6-14, giving a value of 46%. However, in Aspen Plus Radfrac, a plate efficiency was set to 90%, following the heuristic

guidelines, which suggest that tray efficiency for light hydrocarbons from liquid solutions is in the range of 60% to 90%. In this case, a high efficiency value was assumed because using the calculated efficiency, or slightly higher, leads to a drastic increase in the reflux ratio required to achieve 99.9% recovery of propane in the distillate and 99.99% recovery of benzene in the bottoms. Higher reflux ratios increase reboiler and condenser duties, resulting in higher operating and consumption costs.

Table 3.3.3. Internal design of column T-101

UNIT		T-101 Depropanizer column	
Sketch		Column parameters	
	Condenser type		Partial
	Reboiler type		Kettle
	Number of stages		18
	Feed stage		5
	Reflux ratio		10.863
	Distillate rate, kmol/h		12
	Column height, m		9.76
	Column diameter, m		1.55
	Column type		Tray
	Tray type		Sieve
	Material		Stainless steel
Operating conditions			
	Feed	Top	Bottom
Temperature, K	443.17	319.26	486.31

Pressure, bar	15	14.85	15.5
Section CS-1 (stages 2-15)			
	Number of passes	1	
	Tray spacing, m	0.6096	
	Hole diameter, mm	7	
	Hole/Active area	0.06	
	Number of holes	285	
	Side Downcomer Width (Top and Bottom), mm	245.5	
	Side Weir Length, m	1.126	
	Weir Height, mm	50.8	
Downcomer Clearance, mm	30.8		
Section CS-2 (stages 16-32)			
	Number of passes	2	
	Tray spacing, m	0.6096	
	Hole diameter, mm	7	
	Hole/Active area	0.062	
	Number of holes	1592	

		Side Downcomer Width (Top and Bottom), mm	273.7
		Side Weir Length, m	1.182
		Center Downcomer Width (Top and Bottom), mm	291.7
		Weir Height, mm	50.8
		Downcomer Clearance, mm	45
Condenser		Reboiler	
Heat Duty, kW	-556.141	Heat Duty, kW	3116.41

3.3.2 Benzene Column T-102

Overview

Following the depropanizer column, the T-102 benzene column is the second step in the multicomponent separation in the cumene production process. This column is designed to separate benzene from heavier cumene and DIPB, an essential step in obtaining a high-purity cumene product by the end of the separation sequence. High-purity benzene is recovered as an overhead product and recycled back to the process, while the bottom stream, consisting of cumene and DIPB, is sent to the subsequent and last separation unit.

During operation, heat is supplied from the reboiler, causing benzene, the more volatile component, to vaporize and rise through the sieve trays. At the same time, cumene and DIPB remain largely in the liquid phase and flow downward. The overhead benzene vapor is condensed and partially returned as reflux to enhance separation efficiency, while the heavier aromatic mixture is withdrawn from the bottom for further processing.

Type of Design and Operating Conditions for the T-102 Column

The operating conditions of T-102 are based on the zeolite-based cumene production proposed by Norouzi et al. In this process configuration, the bottom product of the depropanizer column is decompressed to 1.3 bar at the valve and then fed to the benzene column [20]. The pressure drop per tray was taken as 0.007 bar in accordance with the tray columns design heuristics by Turton et al [27].

Design and Calculations for T-102 Column

Since the primary goal of the T-102 column is to remove sufficient benzene to guarantee the required 99.9% purity of cumene in the final product stream, the separation fraction of benzene was calculated using the design specification tool in Aspen Plus. Based on that DesignSpec function was created to maintain the amount of benzene in the bottoms flow, which were further used as a basis. For hand and DSTWU calculations, the recovery of benzene in the top product was set to 0.99986 (DesignSpec result), while the recovery of cumene was set to 0.0001. Based on those molar fractions, hand calculations were performed.

Equations 5-14 were used to calculate N_{min} , N , R_{min} , and R . The relative volatility was estimated as the geometric mean between the condenser and reboiler stages. Once the FUG methodology was performed, the theoretical number of stages was determined to be 23, and this value was used in the DSTWU model to generate the corresponding simulation results. A comparison of the hand-calculated FUG results and DSTWU column results is summarized in Table 3.3.4. below:

Table 3.3.4. Comparison of FUG hand calculations and DSTWU results for T-102 column

Parameter	FUG calculations	DSTWU results	Relative error, %
N_{min}	9.047	9.649	6.230
R_{min}	0.218	0.262	16.86
R	0.327	0.361	9.278

Even though the DSTWU model is also based on the FUG shortcut method, Aspen Plus evaluates relative volatility at every tray; meanwhile, when calculations are performed by hand, constant relative volatility is assumed across the column. This difference contributes to the relative errors in Table 3.3.4.

To set up the RadFrac simulation, initially, the number of stages, reflux ratio, and distillate rate were set to the DSTWU simulation results. Then, preliminary internal designs were simulated, and hydraulic results were used to calculate the Murphree efficiency, as described in Appendix C.3. Based on these calculations, the Murphree efficiency is 43.57% for the CS-1 section and 41.61% for the CS-2 section. Since this estimation is rough due to setting the simulation under

ideal conditions, the Murphree efficiency was taken as 50% in accordance with the cumene production described in Turton et al.'s process [27]. According to the heuristics, tray efficiency is typically 50-60% for separating lower-weight aromatics from higher-weight aromatics; therefore, 50% Murphree efficiency is considered a sufficient estimate.

Once efficiency was added, the previous number of stages was insufficient. The optimization of the number of stages is summarized in Table 3.3.5. The feed stage-to-number-of-stages ratio was kept constant. In contrast, the condenser and reboiler duties and the reflux ratio required to maintain 0.999866 benzene recovery were considered for the number of stages optimization. With the increasing number of stages and decreasing reflux ratio, the reboiler and condenser duties can be observed; however, to balance the energy and column material costs, 33 stages were set in the RadFrac simulation. The number of stages may decrease in the subsequent economic optimization report.

Table 3.3.5 Number of trays optimization

N_{stages}	28	33	38	43
N_{feed}	14	16	19	21
Q_C , kW	-49479.3	-25267.4	-16150.0	-14301.9
Q_R , kW	41965.0	17743.6	8605.8	6747.8
RR	4.5513	1.8331	0.8091	0.6011

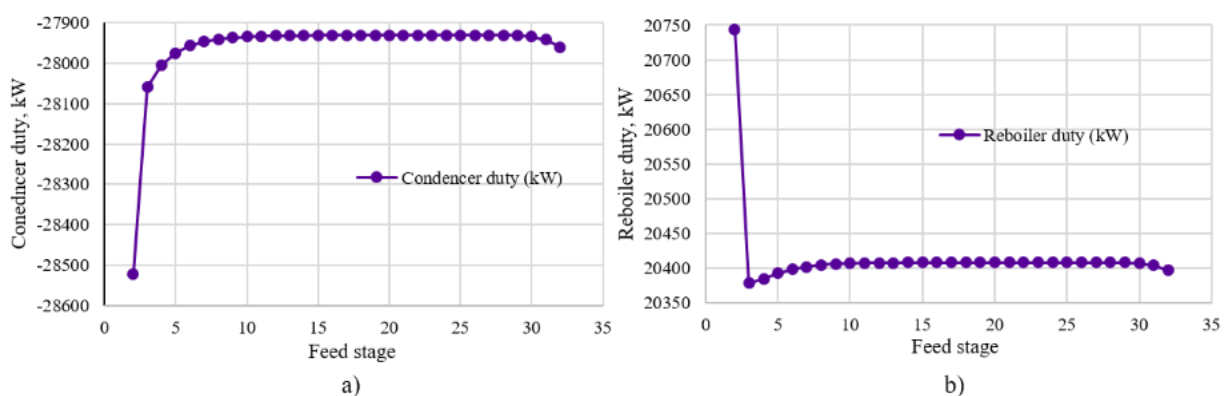


Figure 3.1.3. Feed stage optimization via the evaluation of a) condenser duty, kW and b) reboiler duty, kW

After the number of optimization stages was determined, the feed stage location was analyzed using sensitivity analysis, which evaluated the condenser and reboiler duties once the feed stage was changed. Results of this analysis are shown in Figure 3.3.3. Since the results for

stages below the 16th stage were simulated with errors, and between the 10th and 28th stages heat duties for both the reboiler and condenser are stable the 16 remained as a feed stage. Since the results for stages below the 16th stage were simulated with errors, and between the 10th and 28th stages, heat duties for both the reboiler and condenser are stable, the 16th stage remained as a feed stage.

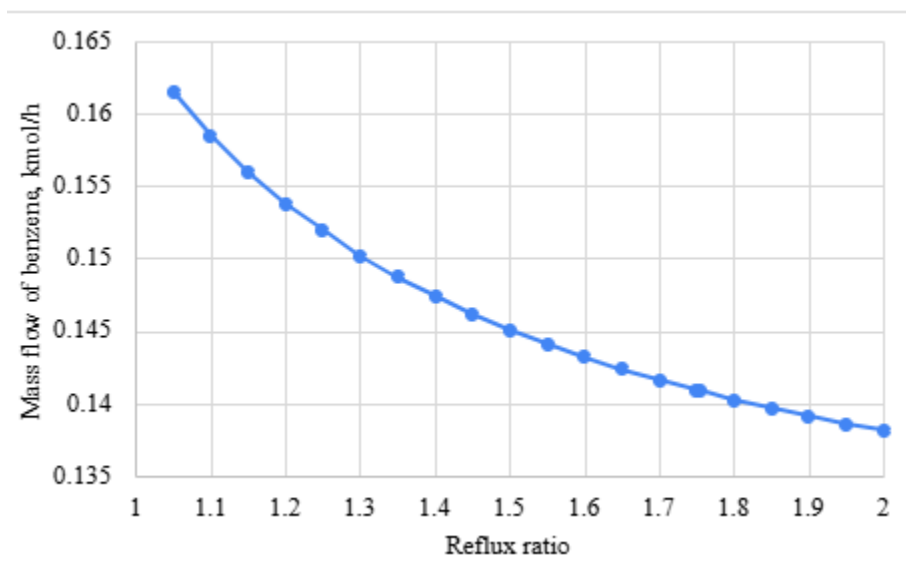


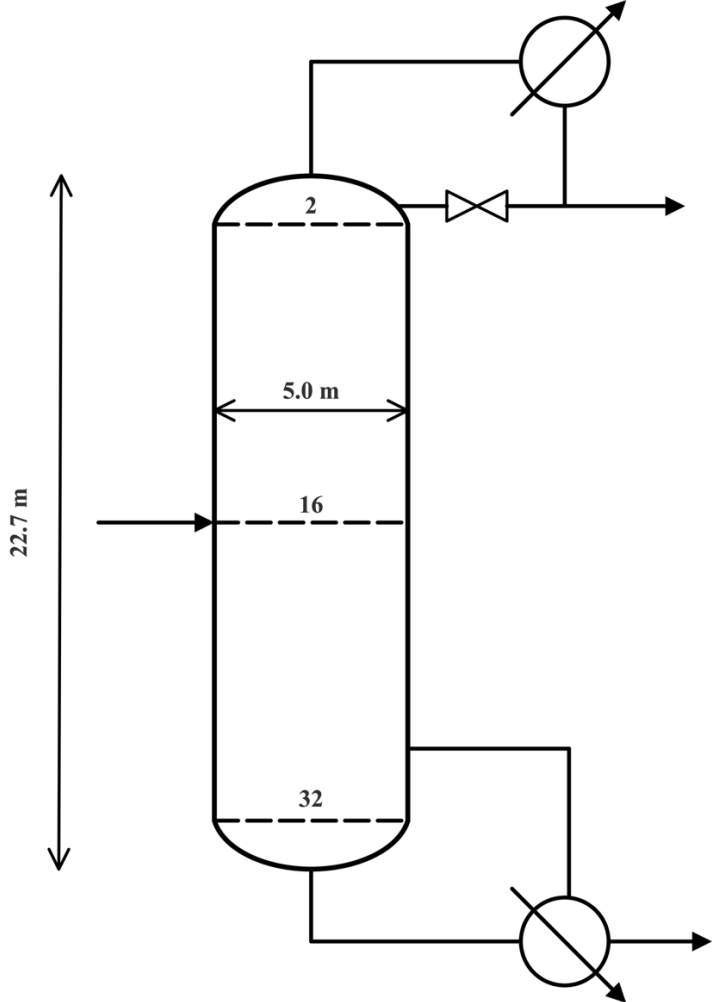
Figure 3.3.2. Benzene flow rate in bottom product vs reflux ratio

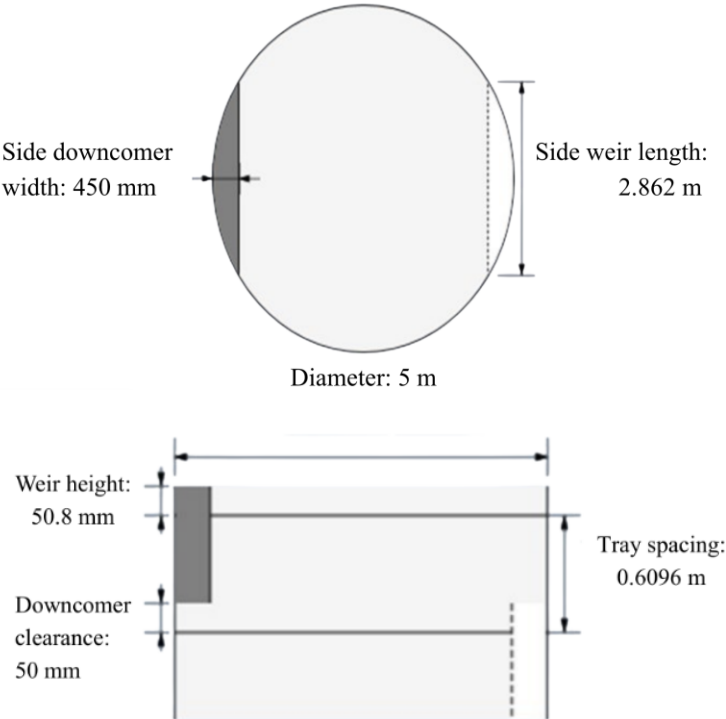
A higher reflux ratio leads to purer distillate. Sensitivity analysis results for the reflux ratio and its impact on the molar flow of benzene in the bottom product of T-102 are shown in Figure 3.3.4. To obtain a cumene purity of 99.9%, a design specification tool was employed, which determined an optimal reflux ratio value of 1.7547. At this value, the fraction of benzene in the distillate is minimized, resulting in benzene recovery of 0.99986. Furthermore, to maintain the lowest possible condenser and reboiler duties, the reflux was set with high precision, obtained from the design specification tool.

T-102 Internals Design

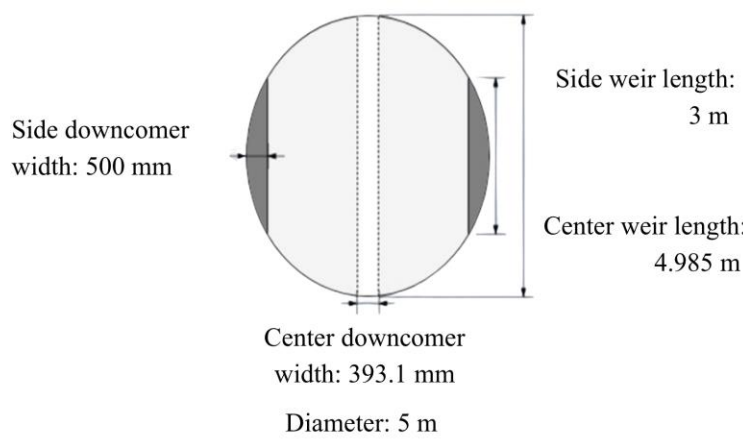
Table 3.3.6. Internal design of column T-102

UNIT	T-102 Benzene column	
Sketch	Column parameters	
	Condenser type	Total
	Reboiler type	Kettle

		Number of stages	33
		Feed stage	16
		Reflux ratio	1.75
		Distillate rate, kmol/h	1063
		Column height, m	22.67
		Column diameter, m	5
		Column type	Tray
		Tray type	Sieve
		Material	Stainless steel SA516 Gr70
Operating conditions			
	Feed	Top	Bottom
Temperature, °C	99.95	85.67	167.18
Pressure, bar	1.3	1.195	1.419
Section CS-1 (stages 2-15)			
		Number of passes	1
		Tray spacing, m	0.6096
		Hole diameter, mm	7
		Hole/Active area	0.1

 Side downcomer width: 450 mm Side weir length: 2.862 m Diameter: 5 m Weir height: 50.8 mm Downcomer clearance: 50 mm Tray spacing: 0.6096 m	Number of holes	46472
	Side Downcomer Width (Top and Bottom), mm	450
	Side Weir Length, m	2.862
	Weir Height, mm	50.8
	Downcomer Clearance, mm	50.0

Section CS-2 (stages 16-32)

 Side downcomer width: 500 mm Side weir length: 3 m Center weir length: 4.985 m Center downcomer width: 393.1 mm Diameter: 5 m	Number of passes	2
	Tray spacing, m	0.6096
	Hole diameter, mm	7
	Hole/Active area	0.08
	Number of holes	32486
	Side Downcomer Width (Top and Bottom), mm	500
	Side Weir Length, m	3
	Center Weir Length, m	4.895
	Center Downcomer	393.1

		Width (Top and Bottom), mm	
		Weir Height (mm)	50.8
		Downcomer Clearance (mm)	50.8
Condenser		Reboiler	
Heat Duty, kW	-32890.9	Heat Duty, kW	25709.5

3.3.3 Cumene Column T-103

Overview

The cumene separation column functions as the final major separation step in multicomponent separation. In addition, traces of benzene present in the feed must be preferentially removed overhead to meet the cumene product specification of 99.9% purity. The column, therefore, performs a cumene/DIPB split while simultaneously polishing light aromatics from the product. The separation relies on the moderate difference in volatility between cumene and DIPB, allowing distillation to concentrate cumene in the vapor phase selectively. The high-purity cumene is collected as the distillate and removed from the system. At the same time, the DIPB/benzene mixture, withdrawn as the bottom product, is mixed with the benzene recycle stream and directed to the R-102 transalkylation reactor for further conversion into cumene. The reactor effluent is then again processed in this column.

Type of Design and Operating Conditions for T-103 Column

Since the cumene separation column is present as the purity-defining step in all major research on the design of the process, in the transalkylation configuration reported by Pathak et al., separation proceeds after light-ends removal and benzene recovery, with the final column producing approximately 99.9 mol% cumene while DIPB is withdrawn as the heavy product [14]. Similar conclusions are reported for conventional designs discussed by Lyuben et al. [33], in which the final separation produces high-purity cumene and rejects DIPB to the bottoms.

As the basis for primary design estimates, the operating conditions listed in the work by Norouzi et al. on the zeolite-based cumene production process were used and modified to account for feed conditions affected by T-102 column modifications [20]. The summary of the adjusted feed conditions and operating parameters is included in Table 3.3.9.

Design and Calculations for T-103 Column

The primary design of column parameters was performed using shortcut methods, followed by validation in Aspen Plus. Analogous to column T-102, the relative volatilities for top, feed, and bottom were estimated using extended Antoine correlation. To apply the FUG method in a multicomponent system, the feed mixture was assumed to be pseudobinary. That is, given the high purity target and the dominance of cumene and DIPB in the mixture, the system was treated as a key-component pair: cumene-LK, P-DIPB-HK. Benzene was treated as a light non-key component present in trace amounts.

The unified relative volatilities for FUG method calculations were taken as the geometric mean of the values at the top and bottom plates. This approach provides a reasonable approximation when temperature variation along the column is moderate. The temperature profile of the T-103 column is presented in Appendix C.3.

Equations 5-14 were used to calculate $N_{\min}$, N , $R_{\min}$, and R . The resulting design basis ($N = 35$) was used as an initial input to the DSTWU column in Aspen Plus, which produced results on $N_{\min}$, $R_{\min}$, and R for comparison with theoretical calculations. The factor for multiplying $R_{\min}$ was chosen from the range 1.05 to 1.5 and selected as 1.5 based on the lowest relative error (2.80%) observed in the Aspen Plus simulation results.

The comparison of the hand calculation results with Aspen Simulation outputs is summarized in Table 3.3.7. below.

Table 3.3.7. Comparison of FUG hand calculations and DSTWU results for T-103 column

Parameter	FUG calculations	DSTWU results	Relative error, %
$N_{\min}$	13.450	14.009	3.99
$R_{\min}$	0.351	0.413	15.13
R ($R = 1.5 R_{\min}$)	0.539	0.541	2.76

Considering a 5% relative difference as an acceptable tolerance, hand calculations for the minimum number of stages and the actual reflux ratio are close to the DSTWU outputs. The 15.13% difference in minimum reflux values is justified, since the Underwood equation order determines the number of equation orders and, therefore, $R_{\min}$ calculations are sensitive to feed thermal condition (q), relative volatilities, and feed composition. Most importantly, the larger deviations are due to assumptions made in the shortcut method at the beginning.

The initial design of T-103 was based on 31 theoretical stages, assuming ideal equilibrium behavior. However, when a uniform Murphree tray efficiency of 50% was introduced, the column could no longer achieve the required distillate purity of 99.9 mol% cumene at the previously selected reflux ratio. To compensate for the reduced stage efficiency, a significantly higher reflux

ratio ($R = 15.5$) was required, which resulted in excessively high condenser and reboiler duties (approximately 24 MW). Such energy consumption is economically unfavorable and runs counter to the objective of minimizing operating costs.

To restore separation performance while reducing energy demand, the total number of stages was incrementally increased. As expected from distillation theory, increasing the number of stages reduces the required reflux ratio for the same separation, thereby decreasing both condenser and reboiler duties. This trend is clearly observed in Table 3.3.8: when the number of stages increases from 31 to 35, the optimal reflux ratio decreases from 15.5 to 1.18, accompanied by a substantial reduction in energy duties. Although the case with 37 stages is the lowest reflux ratio ($R = 0.89$) and slightly lower duties, the marginal energy savings compared to 35 stages are relatively small, while the additional cost associated with extra trays and increased column height becomes significant. Therefore, 35 stages represent the thermodynamically most efficient configuration in terms of energy reduction.

Table 3.3.8. Effect of total stage number on reflux ratio and energy duties for column T-103.

Number of stages, N	Optimal reflux ratio, R	Condenser duty, kW	Reboiler duty, kW	Distillate purity
31	15.5	-23838.8	24575.2	99.99%<
33	2.8	-5490.16	6226.353	
35	1.18	-3151.17	3887.55	
37	0.89	-2730.13	3466.51	

To validate the preliminary design of the cumene purification column, a series of sensitivity studies was performed in Aspen Plus. The purpose was to evaluate the column's separation efficiency with respect to feed-stage location, internal vapor–liquid traffic, temperature distribution, and composition profiles. The results confirm thermodynamic consistency, appropriate hydraulic behavior, and achievement of the target product purity.

Selection of the Optimal Feed Tray Location

A sensitivity study was conducted to evaluate the influence of feed stage location on condenser duty, reboiler duty, and distillate purity for column T-103. The objective was to confirm the thermodynamic optimum feed position and assess the impact of misplacement on energy requirements and separation performance.

As shown in Figure 3.3.5 (a), the reboiler duty exhibits a sharp decrease when the feed stage is moved from the very top of the column to lower stages. Once the feed is positioned within

the optimal region (approximately stages 4-6), the reboiler duty stabilizes and remains nearly constant. Figure 3.3.5 (b) shows a similar trend for condenser duty. As the feed stage moves downward at around the 10th stage, the condenser duty approaches a plateau of approximately -4423.8 kW. According to Figure 3.3.5(c), there is significant variation in distillate purity with feed-stage location. A great improvement in purity is observed when the feed stage is moved towards the 7th stage. After approximately stage 10, the purity reaches a plateau at the target purity of approximately 99.9%, indicating that the column operates in a stable separation region with met specifications after feed is located from stage 15 onward. A more detailed analysis of product purity reveals that only at feed stages 22 and 23 does the target purity hold. Therefore, the optimized feed stage for the column was selected to be 23.

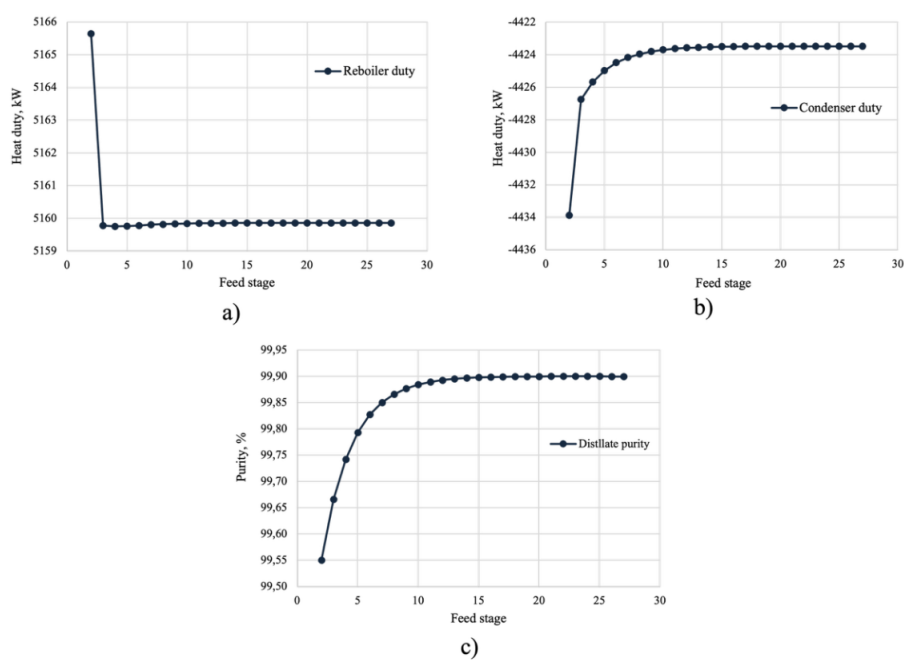


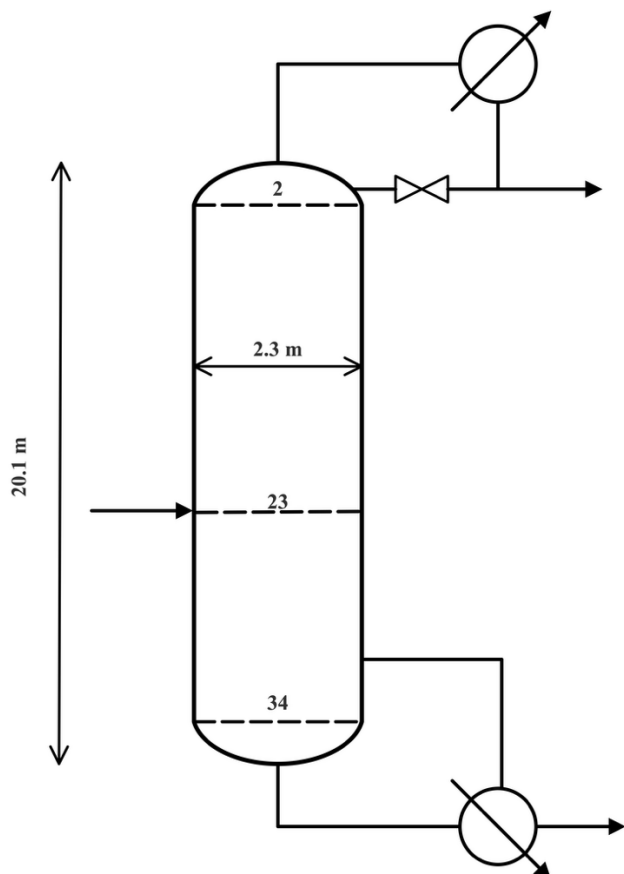
Figure 3.3.1. Sensitivity of (a) Reboiler Duty, (b) Condenser Duty, and (c) Distillate Purity to Feed Stage Location in T-103

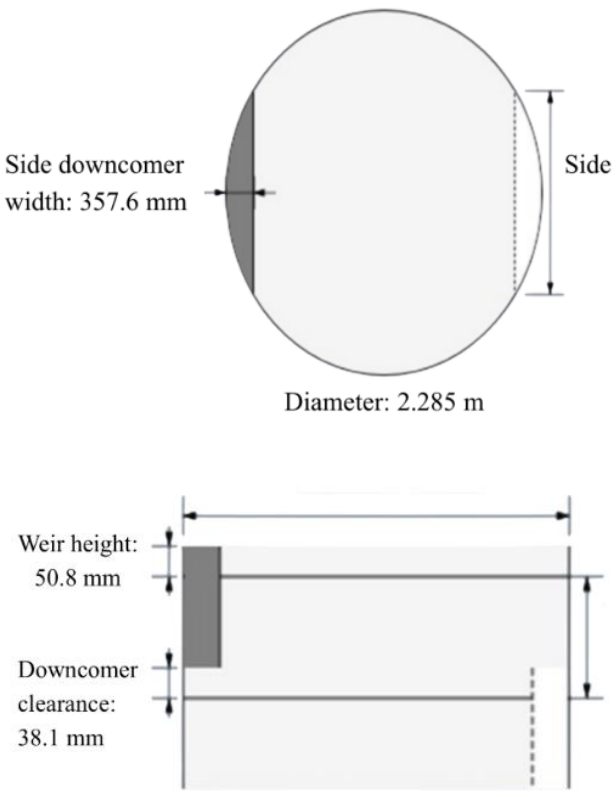
A dedicated sensitivity analysis of the reflux ratio was not performed because the design objective was to determine the minimum reflux ratio that meets the required distillate purity of 99.9 mol% cumene. In distillation design, operating at the lowest reflux ratio that meets the separation specification is economically favorable, as higher reflux directly increases condenser and reboiler duties, thereby increasing operating costs.

Overall, the T-103 column optimization resulted in an increase in cumene purity to 99.9% and a reduction in reboiler heat duty by 20 MW (84% of the initial value), while keeping the reflux ratio at a moderate level.

T-103 Internals Design

Table 3.3.9. Internal design of column T-103

UNIT	T-103 Cumene column		
Sketch	Column parameters		
	Condenser type	Total	
	Reboiler type	Kettle	
	Number of stages	35	
	Feed stage	23	
	Reflux ratio	2.06	
	Distillate rate, kmol/h	142.998	
	Column height, m	20.12	
	Column diameter, m	2.29	
	Column type	Tray	
	Tray type	Sieve	
	Material	Carbon steel SA516 Gr70	
Operating conditions			
	Feed	Top	Bottom
Temperature, K	369.074	435.841	499.213
Pressure, bar	1.419	1.314	1.524
Section CS-1 (stages 2-34)			
	Number of passes	1	
	Tray spacing, m	0.6096	
	Hole diameter, mm	6.0	

	Hole/Active area			0.1
	Number of holes			11606
	Side Downcomer Width (Top and Bottom), mm			357.6
	Side Weir Length, m			1.661
	Weir Height, mm			50.8
	Downcomer Clearance, mm			38.1
Condenser	Reboiler			
Heat Duty, kW	-4423.48	Heat Duty, kW	5159.86	

Chapter 4. Design of Minor Equipment and Storage Tanks

4.1 Design of Minor Equipment

Design of Pumps

In this process, pumps are used to increase the pressure of the streams to meet the units' operating conditions.

Table 4.1.1. Pump specifications

Pump/work	ΔP , bar	Net work, kW (Aspen)
P-101	34	26.47

P-102	34	113.69
P-103	23.5	19.55

Design of Coolers and Heaters

Cooler E-101 is a cooler that causes condensation of propene in the feed by cooling at constant pressure to the saturation temperature, after which liquefaction begins. Its purpose is to ensure that the propene is supplied to the following units under the required operating conditions.

Cooler E103 reduces the reactor effluent temperature from 242.5°C to 170°C before pressure reduction and distillation. The purpose of this is to lower the volatility of benzene and cumene, and to enhance the separation of the light hydrocarbons in the later stages.

Cooler E-104 decreases the temperature of the distillate from the benzene distillation column from 99.96 °C to 25 °C to provide sufficient mixing of recycle benzene and bottoms effluent from the third distillation column in one stream and in another stream between recycle benzene and feed benzene.

Heater E-105 increases the temperature of the mixture of bottom effluent from the cumene distillation column and a fraction of split recycled benzene from the top of the benzene distillation column to the operating temperature of the transalkylation reactor (240°C), ensuring stable operation and consistent reaction rates.

Cooler E-106, installed downstream of the cumene column bottoms, ensures that the stream enters pump P-103 in a fully liquid state.

Table 4.1.2. Summary of temperature changes and heat duties for coolers and the heater.

Coolers		
Unit	ΔT , °C	Heat duty, kW
E-101	-191.80	-1256.6
E-103	-72.48	-4507.3
E-104	-74.96	-11649.2
E-106	-74.96	-36.6
Heater		
E-105	213.48	1516.0

Design of a Compressor

The compressor C-101 was installed to increase the vapor pressure, thereby elevating the saturation temperature. This enables efficient condensation and helps to overcome system pressure losses. It increases the pressure of fresh propylene (a mixture with propane) from 1 bar to 35 bar to enable stable operation.

Table 4.1.3.1 Pressure changers parameters summary

	ΔP , bar	Net work, kW (Aspen)
C-101	34	605.524

4.2 Design of Storage Tanks

Benzene Storage (V-101)

Benzene is the main feed component in the production of cumene. Because it is a volatile liquid, the chemical is stored in a floating-roof storage tank, which can reduce evaporation losses up to 90% [34]. It is made from stainless steel, characterized by high corrosion resistance and good weldability. Since Kazakhstan's domestic production does not meet the total demand, a portion of the required benzene will be imported from China. To account for transportation time and possible supply chain disruptions, a storage period of 20 days is selected.

The volume of the storage tank is based on the volumetric flow rate of the benzene feed, which is calculated from the mass flow rate and density of the stream, both retrieved from Aspen Plus:

$$q_B = \frac{11177.2 \text{ kg/hr}}{872.1 \text{ kg/m}^3} = 12.82 \text{ m}^3/\text{hr}.$$

If the plant operates 8137 hours per year or approximately 22 hours per day, the total volume needed to store benzene for 20 days is:

$$q_B = 12.82 \text{ m}^3/\text{hr} \times 22 \text{ hr/day} \times 20 \text{ days} = 5715 \text{ m}^3.$$

To provide storage capacity and a safety margin, the total tank capacity was taken at 6000 m³. Thus, six storage tanks, each with a capacity of 1000 m³, were selected for benzene storage.

Propylene and Propane Mixture Storage (V-102)

The propylene and propane mixture is a gaseous fluid that needs to be liquefied to ensure efficient storage. Therefore, it will be stored at 20°C and 1.4 MPa in a horizontal pressure vessel, which is designed to withstand higher pressures. It is made from high-performance carbon steel, intended for pressure vessels due to its good weldability and high strength. Since the demand for propene feedstock is met by domestic production, associated logistics are relatively simple. Therefore, the required storage period of the hydrocarbon mixture is shorter than that of benzene, estimated at 10 days.

The densities of the liquefied pure components at given conditions and mass flow rates were retrieved from Aspen Plus, allowing for the calculation of the required vessel capacity:

$$q_P = \frac{\left(\frac{6193.0 \text{ kg/hr}}{515 \text{ kg/m}^3} + \frac{325.9 \text{ kg/hr}}{495 \text{ kg/m}^3} \right)}{6518.9 \text{ kg/hr}} \times 6518.9 \text{ kg/hr} = 12.7 \text{ m}^3/\text{hr},$$

$$V = 12.7 \text{ m}^3/\text{hr} \times 22 \text{ hr/day} \times 10 \text{ days} = 2780 \text{ m}^3.$$

Accounting for the safety margin, the overall required volume is 3000 m³ and hence, the propene and propane mixture will be stored in two 1500 m³ vessels.

Fuel Gas Storage (V-103)

Existing fuel gas consists mainly of propane and propene in gaseous form, and these compounds should be stored in a pressurized vessel due to their low density and high compressibility. For such purposes, ASTM A56 Grade 70 carbon steel is applicable due to its high strength, suitability at moderate temperatures (170 °C), and high-pressure conditions (15 bar) [35]. According to ASME Section VIII, the design is based on the quality factor, allowable stress, and thickness to ensure safe gas storage [36]. Due to high prices, fuel gas storage tanks are small, with limited storage times of 0.5-4 hours.

Volumetric flow rate is used to calculate the design volume of the tank with a safety margin of 10%:

$$q = \frac{\dot{m}}{\rho_{mix}} = \frac{514.54 \frac{\text{kg}}{\text{hr}}}{19 \frac{\text{kg}}{\text{m}^3}} = 27.08 \frac{\text{m}^3}{\text{hr}},$$

$$V_{tank} = q \cdot t_{storage} = 27.08 \frac{\text{m}^3}{\text{hr}} \cdot 1 \text{ hr} = 27.08 \text{ m}^3,$$

$$V_{design} = 1.1 \cdot V_{tank} = 1.1 \cdot 27.08 \text{ m}^3 = 29.79 \text{ m}^3 \approx 30 \text{ m}^3.$$

Cumene Storage (V-104)

Storage tank for final product – cumene - must be contained within an air-free environment to avoid any formation of peroxides. An additional condition is near atmospheric pressure, as it is a flammable liquid with a high boiling point. From an industrial perspective, carbon steel storage tanks are suitable for storing liquid hydrocarbons at low pressure (1.3 bar) in a large volume (7800 m³). According to API 650, ASTM A36 can be used because it has sufficient strength, is easier to weld, and is cheaper to install [37]. To prevent leakage and peroxide formation, fixed-roof tanks can be constructed [35].

The volume of the storage tank is calculated from the volumetric flow by using Aspen Plus data of mass flow rate and density:

The volume of the storage tank is based on the volumetric flow rate of the benzene feed, which is calculated from the mass flow rate and density of the stream, both retrieved from Aspen Plus:

$$q_c = \frac{\dot{m}}{\rho} = \frac{17181.81 \frac{kg}{hr}}{796.64 \frac{kg}{m^3}} = 21.57 \frac{m^3}{hr} = 472.72 \frac{m^3}{day}.$$

Assuming that the storage time of cumene is 15 days, the total volume is:

$$V_{tank} = q_c \cdot t_{storage} = 472.72 \frac{m^3}{day} \cdot 15 days = 7090.78 m^3.$$

With a safety margin of 10%, the final design volume of the storage tank is:

$$V_{design} = 7800 m^3.$$

Chapter 5. Plant Location and Layout

5.1 Plant Location

The selection of a chemical plant location is a critical decision that affects both the economic performance and operational efficiency of the process. An optimal site ensures reliable operation, minimizes costs, and supports safe and sustainable production.



Figure 5.1.1. Plant location (Google Earth screenshot)



Figure 5.1.2. Plant location perimeter (Google Earth screenshot)

The government-regulated Special Economic Zones were given priority when deciding where to locate the factory. The primary reason is that businesses operating in SEZs are exempt from value-added tax, corporate income tax, and customs duties [38].

Additionally, one of the most important factors is the availability of raw materials. Locating the plant close to feedstock sources reduces transportation costs and ensures a stable supply. The chosen location is approximately 5 km from the KPI Petrochemical Complex, which produces propylene, and almost 2 km from the Atyrau Oil Refinery, which produces benzene [39]. Such proximity results in lower logistics costs and higher profit from the final product. Moreover, proximity to markets is also important, as it minimizes the cost of distributing final products and improves overall logistics efficiency.

Moreover, access to transportation infrastructure, such as railways, pipelines, highways, and ports, is essential for the efficient movement of both raw materials and products. In addition, the availability of utilities (electricity, fuel, water) is crucial for continuous plant operation, as a reliable, low-cost utility supply can significantly reduce operating expenses [40]. As can be seen in Figure 5.1.1, the location has access to transportation of roads and railways, as well as proximity to pipelines, given the oil refinery. Furthermore, Figure 5.1.1 depicts the presence of water reservoirs that can be used for plant utility.

Environmental and regulatory requirements must also be considered. The plant location should comply with safety standards and waste management regulations while minimizing environmental impact. The Atyrau region meets environmental and regulatory requirements, as industrial projects in Kazakhstan are subject to strict environmental impact assessments and emission control regulations. In addition, the presence of a well-developed petrochemical cluster provides access to a skilled workforce, supporting efficient plant operation. Therefore, the local labor market is sufficient to provide the new plant with experienced workers. On top of that, the region is highly interested in developing young specialists, so Atyrau Oil and Gas University offers over 100 scholarships every year.

Other criteria to consider include weather conditions. The climatic conditions of the Atyrau region are suitable for plant construction, as the area has a dry continental climate with low precipitation and relatively stable weather. These conditions reduce risks related to corrosion, flooding, and weather-related disruptions, allowing reliable operation and maintenance of industrial facilities throughout the year.

Moreover, the chosen topography is uniform and requires no major changes. The ground is flat and requires no major intervention. Moreover, the location is surrounded by steppes that allow for easy expansion in the future.

5.2 Plant Layout

The plant layout has been designed in accordance with the general guidelines and incorporates essential process safety considerations. As shown in Figure 5.2.1, the layout is organized into distinct functional zones according to their level of risk and operational role.

The red zone corresponds to the main process area and storage tanks. This part presents the highest level of hazard as many reactive substances and high-temperature operations are utilized. The orange zones represent areas associated with equipment and support functions, including utilities, workshops, laboratory, control room, and firestations, where moderate operational risks are present. The green zones indicate low-risk areas, such as administrative buildings, canteen, parking, and auxiliary facilities, including medical services, first-aid units, changing rooms, and sanitary areas. These zones are strategically positioned at a safe distance from hazardous operations to ensure personnel safety.

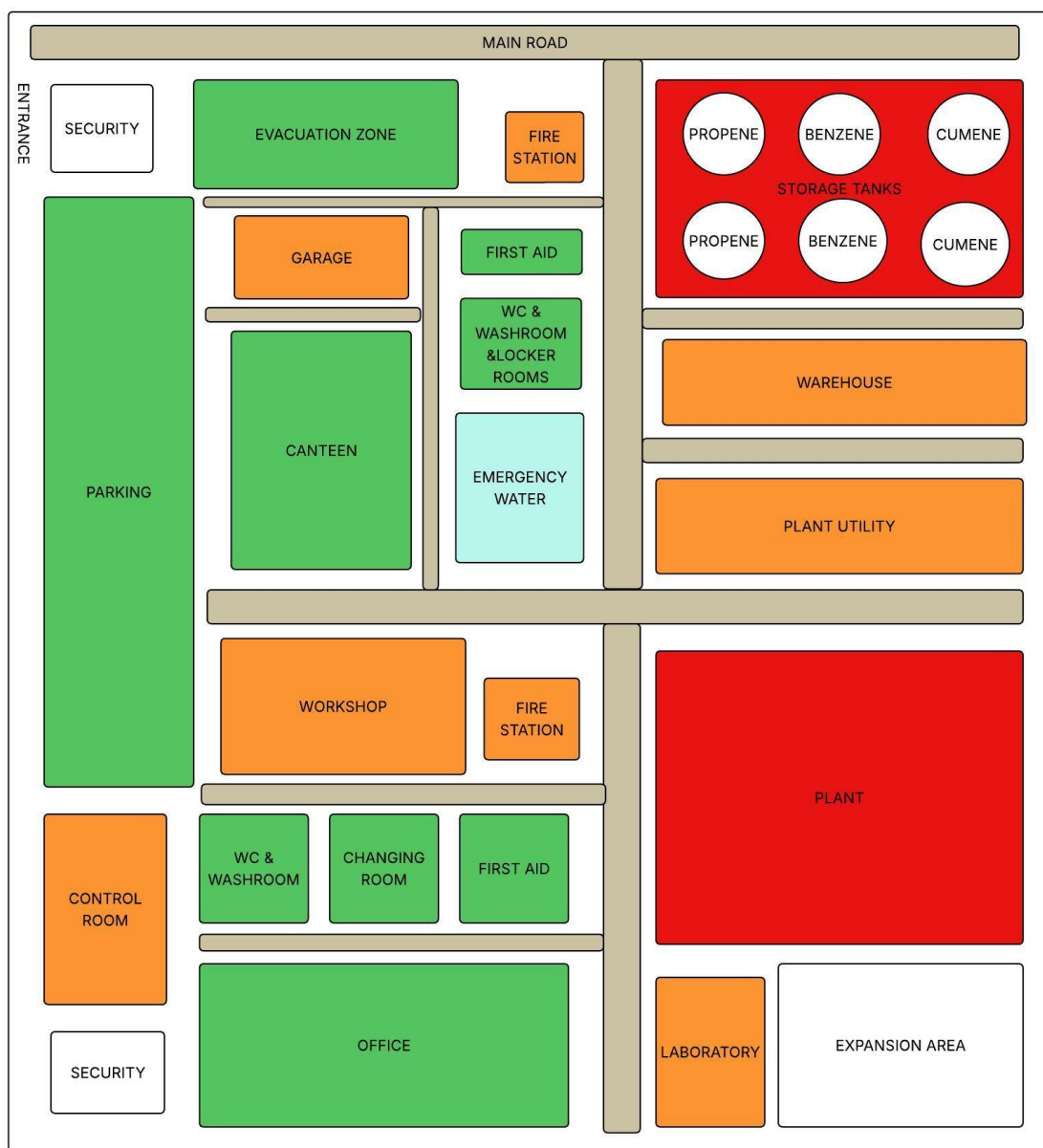


Figure 5.2.1. Plant layout with the indicated risk zones

Storage of raw materials and products is located apart from the main manufacturing area to reduce the risk of large-scale explosions and enhance overall safety. Moreover, for ease of transportation, the storage tanks were positioned closer to the main road, as faster loading and unloading of raw materials and products reduces travel time.

Furthermore, to ensure a rapid response in the event of a disaster, emergency zones (fire station, first aid, emergency water, and evacuation area) are intentionally positioned close to one another. The plant has two security checkpoints at the corners of the plant area, which enhances control and safety.

Parking lots, the canteen, and office buildings are located distant from the primary production zones to minimize exposure to high-risk operations and provide both comfort and safety. Moreover, restrooms and changing areas are located near work areas to promote hygiene. In this way, workers are provided with better working conditions to ensure overall productivity.

To accommodate future growth, the layout incorporates extra space, which offers flexibility to scale production up without interfering with the existing workflow.

Chapter 6. Process Safety and Hazard Analysis

6.1 HAZOP Analysis for Major Units

Table 6.1.1. HAZOP analysis for heat exchanger

Guide Word	Deviation	Causes	Consequences	Actions
NONE	No flow on shell side	Upstream block valve fully closed; P-101 failure	Low conversion.	Temperature indicator, low-temperature alarm
NONE	No flow on tube side	Downstream block valve closed, R-101 shutdown	Cold feed to R-101	High-flow alarm, temperature indicator on reactor inlet
MORE	Higher than design flow rate	Flow controller failure	Lower outlet temperature, feed enters R-101 below design temperature	High-temperature alarm, temperature recorder on stream 7

LESS	Reduced feed flow	Partial blockage, pump P-101 degraded	Lower throughput, possible overheating of feed, increased fouling tendency	Temperature indicator, adjust feed rate to match heating capacity
LESS	Reduced hot-side flow	Partial valve closure, fouling on tube side	Insufficient heating of feed, reduced reactor conversion	Check valve on shell-side inlet, P-101 low-pressure alarm
REVERSE	Reverse flow through exchanger	Loss of pump P-101, upstream pressure higher than downstream	Process fluid flows backward, potential contamination	High-temperature alarm, pressure relief valve on exchanger shell
MORE	Higher outlet temperature than design	Tube-side flow increased, tube fouling	Possible polymerization of benzene/propylene, increased pressure in downstream lines, reduced equipment life	Low-temperature alarm, flow monitoring on tube side, periodic cleaning schedule
LESS	Lower outlet temperature than design	Insufficient hot-side flow	Cold feed to R-101, low conversion, propylene slip through reactor	Pressure safety valve on shell side, high-pressure alarm

Table 6.1.2. HAZOP analysis for reactors

Guide word	Deviation	Causes	Consequences	Actions
MORE OF	High inlet temperature	Excessive preheating, heat exchanger/heater malfunction	Higher reactor peak temperature, catalyst damage	Install high temperature alarms at inlets

LESS OF	Low inlet temperature	Poor preheating, heat exchanger/heater fouling	Low reaction rate, low conversion	Install low temperature alarms at inlets
MORE OF	High reactor temperature	Hot spots, high inlet temperature, maldistribution	Increased rate of DIPB formation, catalyst deactivation, pressure rise	Install high temperature alarms
LESS OF	Low reactor temperature	Low feed temperature, catalyst deactivation	Low conversion, reduced cumene production	Monitor temperature profile and catalyst condition
MORE OF	High pressure drop	Catalyst fouling, coke, tube blockage	Hot spots, reduced output	Install differential pressure indicator with alarm
OTHER THAN	Startup/shutdown instead of normal operation	Rapid feed introduction, wrong startup sequence	Catalyst damage, temperature excursion	Prepare startup/shutdown procedure
NO	No feed to R-102	Pump failure, blocked feed line	No DIPB conversion, low cumene recovery	Install flow indicator with low-feed alarm
MORE THAN	Contaminants in the feed	Corrosion particles, water, sulfur compounds	Catalyst poisoning, lower efficiency, increased pressure drop	Add feed filtration and quality control
MORE THAN	Loss of containment	Tube rupture, flange leak, overpressure	Release of flammable aromatic hydrocarbons, fire hazard	Install hydrocarbon detector and emergency isolation

Table 6.1.3. HAZOP analysis for separation columns

Guide word	Deviation	Causes	Consequences	Actions
NONE	No feed to column	Upstream shutdown, pump failure, line blockage	Column dries out, reboiler may overheat, downstream units are starved,	Low-flow alarm (FAL), sump level alarms, feed flow control, startup/shutdown procedure
MORE	Higher than design feed	Upstream throughput increase	Reduced separation efficiency, off-spec downstream streams	High-flow alarm, level control, overhead/bottom composition monitoring
LESS	Lower than design feed	Partial valve closure, upstream upset, pump degradation,	Reduced throughput, unstable temperature profile,	Low-flow alarm, temperature profile monitoring,
MORE	Reboiler temperature too high	Steam control valve failure open, steam pressure surge, dry reboiler	Excessive vaporization, flooding, thermal degradation,	High-temperature alarm, steam flow controller with high alarm,
LESS	Reboiler temperature too low	Steam supply failure, steam valve closed, low steam pressure, fouled reboiler	Insufficient vaporization, inadequate separation,	Low-temperature alarm, composition analyzer,
MORE	Column over-pressure	Condenser cooling-water failure, overhead valve closed,	Vapor release, loss of separation efficiency, fire/explosion hazard,	High-pressure alarm, condenser cooling-water flow alarm,
LESS	Column under-pressure	Excessive condenser duty,	Flammable/explosive	Low-pressure alarm, pressure

		pressure controller failure open	atmosphere, structural damage	controller low limit, inert gas blanket,
NONE	Loss of reflux or condenser failure	Cooling-water failure, reflux pump failure,	Overhead vapors not condensed, separation failure	Cooling-water flow alarm, reflux drum level alarm
MORE	High liquid level in drum	Bottoms pump failure, high feed rate, downstream blockage	Reduced efficiency, flooding from bottom	High-level alarm, pump discharge pressure alarm,
LESS	Low liquid level	High bottoms draw, low feed, reboiler leak, level controller malfunction	Dry reboiler, tube overheating, fire hazard	Low-level alarm, bottoms flow control
PART OF	Poor separation	Insufficient reflux, wrong reflux ratio, low reboiler duty	Loss of product purity, reduced yield, recycle contamination, downstream reactor upset, economic loss	Reflux ratio control, temperature profile monitoring
OTHER THAN	Tray fouling, damage, or abnormal internal condition	Polymer/coke deposits, corrosion	Reduced capacity, poor separation,	Differential-pressure monitoring, cleaning protocol

6.2 Waste streams and Environment

In the present plant design, no waste streams are generated, and therefore, no significant environmental risks are expected during normal operation. The catalyst employed in the production, zeolite- β , is fixed within the reactor and is not discharged with the process streams. Additionally, it is an aluminosilicate material, which in itself does not pose any environmental hazards under operating conditions.

Chapter 7. Economic Evaluation and Cost Analysis

APEA and calculations and estimations are shown in 'economics.xls' ESI file.

7.1 Equipment Costs

The costs of reactors were manually calculated using economic correlations for tubes and the reactor shell [41]:

$$C_{tube} = N_{tubes} \times 6000 \times \frac{(Volume, m^3)(Diameter, cm)^{-1.5}}{0.015} \quad (21)$$

$$C_{shell} = 100000 \times \left(\frac{mass_{shell}}{8000} \right)^{0.58} \quad (22)$$

Cost correlation in Equation 21 already includes the installation factor, whereas the installed cost of the shell is:

$$C_{inst,shell} = C_{shell} \times 2.3 \quad (23)$$

Location factor calculations

The chosen reference point is Shenzhen, China. Location factor for indigenous production in China is 0.61. As a rule of thumb, this factor changes by 10% for every 1000 miles [8]. Considering that the reference point is approximately 5535 miles away from Atyrau:

$$LF_{Atyrau} = 0.61 \times \left(1 + 0.1 \times \frac{5535}{1000} \right) = 0.95$$

Cost escalation

The correlations used in the calculation of reactor cost are based on data from 2007 (CEPCI Index = 525.4). To account for the cost escalation as of 2025 (CEPCI Index = 816.2), the factor is calculated as the following [42], [43]:

$$Cost_{2025} = Cost_{2007} \times \frac{816.2}{525.4} \quad (24)$$

Table 7.1.1. Cost of equipment

Equipment type	Code	Equipment cost, USD	Installation USD	Capital cost, USD
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Heat Exchanger	E-102	46600	132100	832000
Reactors	R-101	670000	745000	1097000
	R-102	550000	539000	901000
Columns	T-101	453900	618900	2760000
	T-102	1985300	1632500	5240000
	T-103	674700	888500	3230000

Table 7.1.2. Cost of storage tanks

Code	Volume, m ³	Number of tanks	Mass of one tank, kg	Total cost, USD
V-101	6000	6	31000	282000
V-102	3000	2	185000	315000
V-103	30	1	9000	106000
V-104	7800	1	137000	441000

7.2 Prices of Final Products

Approximate pricing of raw materials and products is essential for evaluating the economic viability of the cumene production process. Market prices were obtained from two independent commodity pricing sources - ChemAnalyst to ensure reliability and consistency of the estimates.

The process requires two raw material streams: benzene and a propylene-propane mixture. The primary product of the plant is cumene (isopropylbenzene). In addition, the exhaust gas stream recovered from the first separation unit - comprising unreacted propylene and residual propane - is sold as a fuel gas by-product, contributing to the overall revenue of the process. The composition and flow rates of these streams are detailed in the process flow diagram (see Chapter 2).

Table 7.2.1. Product revenue calculation summary

Material	Mass flow, kg/h	Price, USD/tonne	Price, USD/year	Revenue, USD/year
Cumene	17182	910	127379528	129475699
Fuel gas	515	500	2096172	

7.3 Fixed Capital Investment Estimation

Fixed capital investment (FCI) represents the total expenditure associated with the design, construction, and installation of the plant, including all required modifications to the plant site. It consists of four main components: the inside battery limits (ISBL); offsite battery limits (OSBL) investments; engineering and construction costs; and contingency charges [8]. ISBL investment covers all direct costs of the process plant, including equipment purchase, piping, instrumentation, and civil works. It was estimated using the following capacity-based correlation:

$$C_2 = aS_2^n \quad (25)$$

Where C_2 is the ISBL capital cost (million USD); S_2 is the plant capacity (kmol/h), and a , n are cumene production specific parameters taken from the process costs correlations in [8].

OSBL investment accounts for site infrastructure modifications, such as storage and auxiliary facilities. Engineering and construction costs cover design, construction services, and contractor fees. Contingency allowances are included to account for unforeseen expenses during construction. The percentage-based estimates for each component follow standard industry heuristic approximations.

Table 7.3.1. FCI components

Component	Basis	Cost, USD
ISBL	From eq. (25)	25044940
OSBL	40% of ISBL	10017976
Engineering & Construction	10% of (ISBL + OSBL)	3506292
Contingency	10% of (ISBL + OSBL)	3506292
Total		42075499

7.4 Fixed Operating Costs

Operating Labor Cost Estimation

Alkhatat and Gerrard proposed correlation for the estimation of the cost of operating labor [27]. In this correlation, N_{ol} represents the number of operators required per shift, P is the number of processing steps involving particulate solids, and N_{np} is the number of non-particulate

processing steps. For cumene production, $P = 0$, since no solid handling is required. The correlation is expressed as:

$$N_{ol} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (26)$$

The number of non-particulate processing steps, N_{np} , was determined based on the total number of major equipment units in the plant. Valves and pumps were excluded due to their relatively low cost. The total number of relevant equipment units was calculated as 11 by using Equation 26 and is shown in Table 7.4.1.

$$N_{np} = \sum \text{Equipment use} \quad (27)$$

Table 7.4.1. Number of equipment in a plant.

Equipment type	Number of equipment	N_{np}
Heat exchanger	1	1
Reactor	2	2
Distillation column	3	3
Heater	4	4
Pump	3	-
Compressor	1	1
Valve	2	-
Total	16	11

According to [8], a large continuous fluid-processing plant requires three operators per shift: one inside the plant, one outside, and one in the tank farm. The plant operates continuously for 365 days per year, resulting in 1095 shifts annually (3 shifts per day). Each operator works 8-hour shifts for 49 weeks per year (accounting for vacation and sick leave), which corresponds to 245 shifts per operator per year. Therefore, the number of operators required to cover all shifts is $(1095 \text{ shifts/year}) / (245 \text{ shifts/operator/year}) = 4.469$ operators, which is approximately 4.5 operators.

The total operating labor requirement is then calculated using:

$$\text{Operating labor} = N_{ol} \cdot N_{np} \quad (28)$$

which gives a total of 14 operators (rounded to the nearest integer). The average annual salary of a chemical plant operator in the region is approximately 14,880 USD [44]. Therefore, the annual cost of operating labor is:

$$C_{ol} = \text{Operating labor} \cdot \text{Average salary} \quad (29)$$

The major components of the fixed cost of production are summarized in Table 7.4.2. Besides operating labor (from Eq. 28) and supervision, direct salary overhead, which covers non-salary employee benefits such as health insurance, was also estimated and added to the fixed cost of production value. Maintenance encompasses both labor and materials, as well as general plant overhead, which includes shared corporate functions including human resources, R&D, IT, and finance are also components of fixed cost of production.

Property taxes and rent are waived under applicable law and are therefore set to zero, as the plant is located within a Special Economic Zone (SEZ) in Kazakhstan. Meanwhile, environmental charges are assessed on CO₂ emissions, which applies 5 Kazakhstani Monthly Calculation Index (MCI) units per tonne of CO₂ emitted above the set limit not compensated by acquired quota and/or carbon units (Article 329 of the Code of Administrative Offenses of the Republic of Kazakhstan) [45].

Table 7.4.2. Fixed cost of production estimation

Component	Basis	Cost, USD
Fixed capital investment	From table 7.3.1.	42075499
Cost of operating labor	$N_{ol} \cdot \text{average salary}$	208320
Supervision	25% of operating labor	52080
Direct salary overhead	60% of (operating labor + supervision)	156240
Environmental charges	Based on pollution taxes	3551517
Maintenance	3% of ISBL	1252247

General plant overhead	65% of (operating labor + supervision + direct salary overhead + maintenance)	1084777
Total cost (USD)		6305181

7.5 Variable Cost of Production

Cost of Raw Materials

Table 7.5.1. Raw material cost summary

Material	Mass flow, kg/h	Price, USD/tonne	Price, USD/year	Revenue, USD/year
Benzene	11177.2	774	70479212	94378257
Propene (95wt%) + Propane(5wt%)	6519	450	23899045	

Cost of Utilities

Utility costs were estimated using the Aspen Economics tool. The main utilities identified for the process were electricity, cooling water, and steam. Their costs were determined based on the utility consumption requirements of both major and minor equipment throughout the plant. For the specified region of the plant, the price of steam was taken as 13.45 USD/Gcal (calculations are shown in Appendix D), electricity as 0.083 USD/kWh [46], and cooling water as 0.26 USD/tonne [47]. These values were used to quantify the overall utility expenses, which were then incorporated into the operating cost analysis as an essential component of the process economics.

7.6 Economic Analysis

Profit Estimation

Based on the fixed capital investment summarised in Table 7.3.1. and the plant capacity established in Section 1 (Market Analysis), the profitability of the process was evaluated on a first-year basis. A working capital allowance of USD 5.3 million was additionally committed at start-up. Applying the product prices and feed costs tabulated above yields a first-year revenue of USD 142.9 million and a gross profit of USD 23.9 million. Subtracting variable utility costs, the fixed production costs detailed in Table 7.4.2., and depreciation gives an EBIT of USD 22.9 million. After the 20% corporate income tax, net income is USD 13.0 million, and adding back depreciation

yields a first-year net cash flow of USD 14.1 million. Subsequent years were escalated at 10.4% per annum.

7.7 Financial Performance Indicators and Feasibility

The economic viability of the proposed cumene production plant was assessed through a discounted cash flow analysis spanning a 20-year operating horizon from 2027 to 2046, following construction completion in 2026. A nominal weighted average cost of capital of 12% was adopted as the discount rate, with cash flows escalated at an annual inflation rate of 10.4% reflecting Kazakhstan's current macroeconomic environment. The fixed capital investment, estimated at USD 42.1 million using the factored cost method with CEPCI adjustment to 2026 prices, covers ISBL and OSBL costs together with engineering and contingency allowances. Revenue is driven by a plant capacity of 140,020 tons per year of cumene, supplemented by propane/propene fuel gas as a co-product, while operating costs comprise raw materials, utilities, fixed costs, and 20% corporate income tax.

The principal financial indicators (Net Present Value, Internal Rate of Return, cumulative cash flow, and payback period) were evaluated to characterize the project's profitability and risk profile. A summary of these indicators is presented in 7.7.1, while the NPV profile and cumulative cash flow behavior are illustrated in Figures 7.7.1 and 7.7.2.

Table 7.7.1. Summary of key financial indicators

Indicator	Value
Fixed capital investment, USD million	42.1
Net Present Value, USD million	192.5
Internal Rate of Return, %	41.4
Simple payback period, years	3.1
Discounted payback period, years	3.9

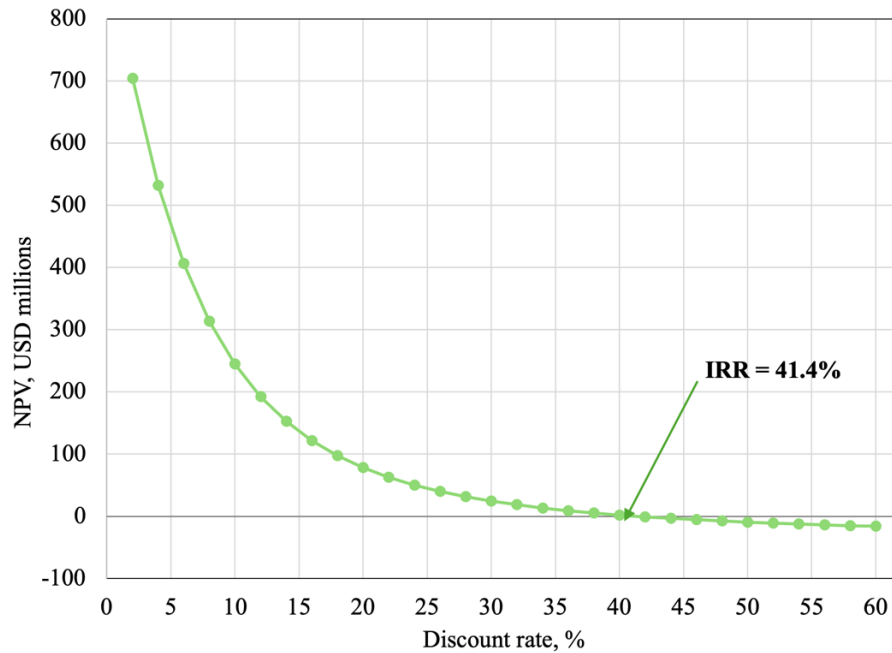


Figure 7.7.1. NPV over different discount rates

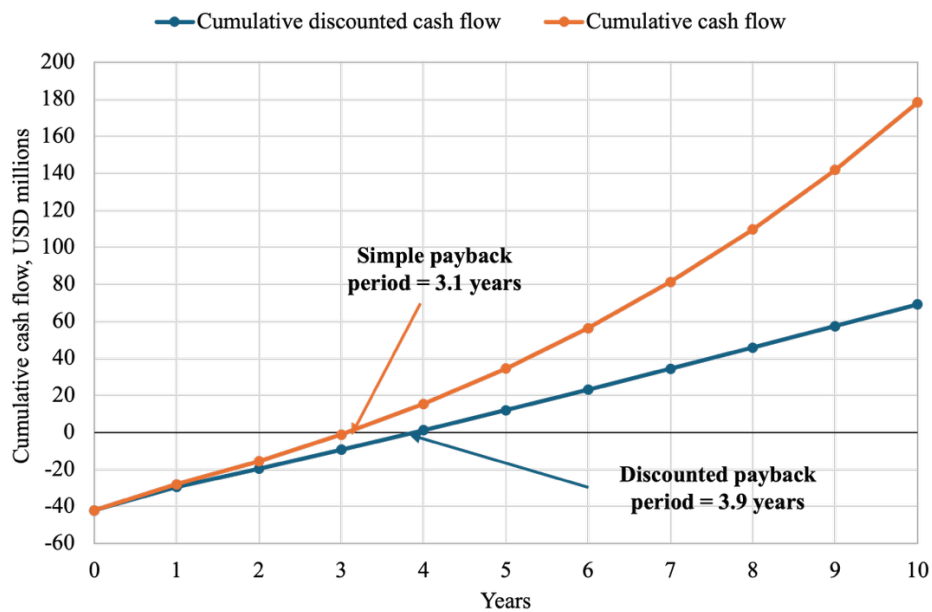


Figure 7.7.2. Cumulative cash flow behavior and payback period

The results demonstrate that the project is economically attractive under the base-case assumptions. A Net Present Value of USD 192.5 million at the 12% discount rate confirms that the venture is expected to generate considerable value over its operating life, and an Internal Rate of Return of 41.4%, which is nearly three and a half times the assumed cost of capital, indicates a

substantial margin of safety against adverse movements in financing costs or cash flows. The simple payback period of 3.1 years and the discounted payback period of approximately 3.9 years both fall well within the project horizon, suggesting that the initial capital outlay can be recovered rapidly and that the remaining sixteen years of operation contribute almost entirely to value creation. Taken together, these indicators support the conclusion that the cumene plant is financially viable and represents a sound investment opportunity, provided that the underlying assumptions on product pricing, raw material costs, and operating performance are realized in practice.

Chapter 8. Conclusions and Future Work

In this project, a complete design of a cumene production plant was developed based on the alkylation of benzene with propylene and subsequent transalkylation of DIPB. The selected process demonstrated high propylene conversion of 99% and improved product yield due to DIPB being converted back via transalkylation. This reduced by-product formation as well as utilization of zeolite-based catalysts.

Detailed process simulation and equipment design confirmed that the system can operate efficiently under the chosen conditions. The results demonstrate a good agreement between manual calculations and Aspen simulations. The design of major units, including reactors, heat exchangers, and separation columns, ensured that the required product purity of 99.7% and production capacity of 140 020 tons/year were achieved.

The plant layout and location analysis indicated that the Atyrau region is the most suitable site due to its proximity to benzene and propylene production facilities, developed infrastructure, and favorable economic conditions. Safety and environmental considerations were incorporated through proper zoning, hazard analysis, and waste management strategies.

Overall, the proposed design is technically feasible, economically viable, and meets modern industrial and environmental standards. Future improvements may include process optimization through enhanced heat recovery to reduce dependency on utility. In addition, the use of more efficient or modified catalysts may further increase selectivity by reducing by-product formation and catalyst deactivation. Environmental contamination can be combatted by optimizing the waste handling process and reusing the waste products as an extra energy source.

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Appendix A. Table of contributions

Section	Topic	Inzhu Turaliyeva	Irada Kazbekova	Aruzhan Baitokova	Alina Komkova	Indira Kairzhanova	Aliya Madaniyetova
Chapter 1: Process Introduction							
1.1	Physical and Chemical Properties	1 st					
1.2	Cumene Applications	1 st					
1.3	Market Analysis		1 st				
1.4	Process Selection			1 st			
1.5	Selection of Catalyst			1 st	1 st		
1.6	Chemical Reaction Mechanism				1 st		
Chapter 2: Process Description							
2.1	PFD, Stream tables and Material Balance		1 st	1 st		1 st	

2.2	Kinetics				1 st		1 st
Chapter 3. Major Units Calculations							
3.1	Design of Heat Exchanger E-102	1 st					
3.2	Design of Reactors R-102 and R-102				1 st		1 st
3.3	Design of Distillation Columns T-101, T-102, and T-103		1 st	1 st		1 st	
3.3.1	Depropanizer T-101			1 st			
3.3.2	Benzene Column T-102		1 st				
3.3.3	Cumene Column T-103					1 st	
Chapter 4: Design of Minor Equipment and Storage Tanks							

4.1	Design of Minor Equipment	1 st	1 st	1 st	1 st	1 st	1 st
4.2	Design of Storage tanks				1 st		1 st
Chapter 5: Plant Location and Layout							
5.1	Plant location	1 st					
5.2	Plant layout	1 st					
Chapter 6: Process Safety and Hazard Analysis							
6.1	HAZOP Analysis for Major Units	1 st	1 st	1 st	1 st	1 st	1 st
6.2	Waste streams and Environment				1 st		
Chapter 7: Economic Evaluation and Cost Analysis							
7.1	Equipment costs	1 st	1 st	1 st	1 st	1 st	1 st
7.2	Prices of Final Products		1 st				

7.3	Fixed Capital Investment Estimation		1 st				
7.4	Fixed Operating Costs		1 st	1 st			
7.5	Variable Cost of Production			1 st		1 st	
7.6	Economic Analysis			1 st		1 st	
7.7	Financial Performance Indicators and Feasibility			1 st		1 st	
Chapter 8: Conclusions and Future Work							
8.1	Conclusions and Future Work	1 st					

Appendix B. Chapters 1 & 2

Appendix B.1. Market analysis

Plant production capacity estimation and feedstock availability

The estimation by GDP will be used in further estimation, as GDP is a more suitable parameter for economic estimations, as it reflects the size of the economy and industrial base. Taking 25% of this estimate yields ~235,000 metric tons per year, which aligns with typical plant

capacity ranges described in Chemical Engineering Design, Chapter 6 [1]. However, there are certain limitations associated with the feedstock availability in the region.

The main problem of feedstock deficiency is associated with the lack of benzene production in Kazakhstan, as the sole producer in Kazakhstan is the Atyrau Oil Refinery, with an annual output of about 55 thousand metric tons while to produce 235,000 metric tons of cumene per year 154,000 metric tons of benzene is required [2]. Meanwhile, the propylene production in Kazakhstan meets the demand for cumene production, as KPI Inc. manufactures approximately 500 million metric tons of polypropylene annually from raw propylene [3].

Due to the fact that the demand for benzene is not met, the plant capacity is reduced to the smallest possible value, which is reported in the Chemical Engineering Design, Chapter 6 - 140,000 metric tons per year. For this amount of cumene, only 92,000 metric tons per year of benzene is required. The rest of the required benzene will be bought from China, as it produces about 19 million metric tons of benzene per year [4].

Chemical specifications for a product and reactants

The desired purity of produced cumene is 99.9% (w/w), as it is the required specification for the primary application of cumene, which is phenol and acetone production [5]. The rest - 0.1 % (w/w) is usually the side product - DIPB or unreacted benzene or propylene [6].

Benzene used in the cumene production is required to be a high-purity chemical, whose composition is about 99.985 % (w/w), with less than 0.015 % of impurities [7]. The major impurity in benzene is C6 and C7 nonaromatic hydrocarbons, and water [8].

Meanwhile, the required propylene purity is a little lower, usually about 99.5 % (w/w) [8]. In cumene production, the propylene stream is usually diluted with 0.5 mol% of propane, which acts as an inert compound in the process [6]. To estimate other possible impurities in the propylene stream, Chevron Phillips Chemical Company's pipeline specifications were evaluated: the rest of the allowed impurities are usually about 500 ppm mol of methane and ethane mixture, with insignificant amounts of other chemicals such as hydrogen (20 ppm mol), ethylene (15 ppm mol), water (12 ppm mol), etc. [9]. Unsaturated hydrocarbons are chemicals, which exceeded amount can cause the biggest disturbance in the process, as they compete with propylene in reactions with benzene, and form side-products which are harder to separate [8].

Profit and expenses estimation

The average selling price for cumene will be about one in Asia, which is about USD 910 per metric ton [10]. Meanwhile, propylene is estimated to be around USD 876/MT (Qingdao, China) and Kazakhstan's benzene exports in 2024 were USD 435/MT [11, 12]. Based on these average market prices and values of benzene and propylene per tonne of cumene estimated on Figure B.1.1, profit per MT of cumene is USD 315.

Table 6.3 Overall process material balance after Dow-Kellog technology [3].

Material	kg/ton cumene	Utilities	Per metric ton cumene
Feed:			
Benzene (100%)	653	Fuel for heating purposes (hot oil, steam, fired reboiler)	0.60 Gcal
Propylene (100%)	352	Steam (export) as LP at 3.5 atm	525 kg
Product	1000	Cooling water at maximum cooling air	1.08 m ³
Cumene			
Heavies	6	Electricity	17.0 kWh
LPG	variable		

Figure B.1.1. Material balance and approximate utilities expenses. Retrieved from [13].

Calculation of utility costs:

$$17 \text{ kWh} \cdot 0.066 \frac{\text{USD}}{\text{kWh}} [14] = 1.12 \text{ USD electricity cost}$$

$$17 \text{ m}^3 \cdot 1.31 \frac{\text{USD}}{\text{m}^3} [15] = 1.12 \text{ USD water cost}$$

$$0.60 \text{ Gcal} \cdot 11 \frac{\text{USD}}{\text{Gcal}} [16] = 6.6 \text{ USD cost for gas}$$

$$\text{Total cost} = \text{electricity cost} + \text{water cost} + \text{cost for gas} = 9.12 \text{ USD (B.1.1)}$$

Plant capacity

An average annual rate of growth of demand for acetone is 4.2%

During the acetone and phenol production, 25% of acetone is created for cumene; therefore, the preliminary annual growth for cumene is 16.8%, see calculation below.

$$\frac{4.2\%}{0.25} = 16.8\%$$

Since 95% of cumene is used for phenol and acetone production, 17.7% is the final annual growth for cumene.

$$\frac{16.8\%}{0.95} = 17.7\%$$

Demand for cumene in 2022 is 17 million MT, current demand is estimated below:

$$17 \text{ million MT} \cdot (1 + 0.177)^{2025-2022} = 17 \text{ million MT} \cdot (1 + 0.177)^3 = 27.72 \text{ million MT}$$

Demand for cumene in 10 years, in 2035:

$$17 \text{ million MT} \cdot (1 + 0.177)^{13} = 141.43 \text{ million MT}$$

Demand for Mainland China:

$$27.72 \text{ million MT} \cdot 0.25 = 6.93 \text{ million MT}$$

Scaling down demand for CIS region by GDP:

$$6.93 \text{ million MT} \cdot \frac{2.8 \text{ trillion USD}}{19.2 \text{ trillion USD}} = 1.01 \text{ million MT}$$

Scaling down demand for CIS region by population:

$$6.93 \text{ million MT} \cdot \frac{251.8 \text{ million}}{1400 \text{ million}} = 1.25 \text{ million MT}$$

25% of CIS region:

$$25\% \cdot 1.01 \text{ million MT} = 253 \text{ thousand MT}$$

Due to unavailability of feedstock, plant capacity will be estimated from the lowest production production rate:

Production per hour:

$$140000 \frac{\text{MT}}{\text{year}} \cdot \frac{1 \text{ year}}{365 \text{ d}} \cdot \frac{1 \text{ d}}{24 \text{ h}} \cdot \frac{1}{0.93(\text{on-stream factor})} = 17.2 \frac{\text{MT}}{\text{h}} = 172000 \frac{\text{kg}}{\text{h}} = 143 \frac{\text{kmol}}{\text{h}}$$

143 kmol/h is selected as the required production rate for mass balance calculations.

Appendix B.2. Catalyst comparison

Table B.2.1. Comparative table of catalysts used in the manufacturing of cumene

Catalyst	Description	Operating	Yield/Selectivity	Pros	Cons

		conditions			
SPA [17, 18, 19]	A mixture of polyphosphoric acid, pyrosiliconphosphate, and orthosiliconphosphate mixture supported on kieselguhr. Licensed by UOP. Fixed-bed reactor, gas phase.	T: 180-260 °C P: 3-4 MPa Benzene: Propylene ratio: 5-7	About 94-95 wt.% cumene	Propylene conversion in one pass, simple	Yield is limited to 95%, heavy by-products production, non-regenerative, and short life of the catalyst, corrosive
AlCl ₃ [18, 19, 20, 21]	Homogeneous liquid-phase catalyst.	T: lower than 135 °C P: lower than 0.4 MPa Benzene: Propylene ratio: lower than SPA	About 98-99 wt.% cumene	High cumene yields, operation at mild conditions, transalkylation	Corrosion issues, catalyst separation needs water/caustic washing, environmentally hazardous, and production of undesired n-propylbenzene
Zeolite-based [22, 23]	Heterogeneous, solid catalyst. Employed by CDTech (liquid-phase process), UOP, Mobil-Badger, Enichem, and Dow.	T: 170 °C P: 3.6 MPa Benzene: Propylene ratio: controlled through	Cumene product purity: 99.5%	High yield, regenerable catalyst, no corrosion concerns, safe disposal, and low-cost maintenance	Complex process, performance varies by licensor

		benzene recycle			
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Table B.2.2. Summary of properties of different zeolites

Type of zeolite	Patented by	Structure	Si/Al ratio	Stability	Conditions
MCM-22 [24, 25]	Mobil Oil Corp. (US4954325)	Layered structure with 10 and 12-membered rings located between the layer and “cups” on the external surface	10-30	Thermally stable	T: 10-125°C P: 1-30 atm.
Zeolite-β [25, 26]	Mobil Oil AS (US3308069)	12-membered ring, low micropore volume and large mesopore volume	10-100	Thermally stable from 20°C up to 500°C	Relatively low temperatures and small amounts of catalyst
ZSM-5 [27, 28]	Mobil Oil AS, ExxonMobil Corp. (US3702886)	Three-dimensional framework consisting of chains of eight 5-membered rings	5-100, preferred 10-40	Should be incorporated with another material resistant to thermal effects	Preferred temperature range is 150-175°C

Table B.2.3. Comparison of zeolite-based catalysts in the production of cumene

Type	Pros	Cons
Zeolite-β [25, 29]	Low steric hindrance within the ring, allowing benzene and cumene to diffuse without difficulty	Susceptible to deactivation when B/P ratio decreases from 7.2 to 3.5

	Large pores allow for better performance without deactivation due to the formation of high-molecular hydrocarbons	Greater formation of DIPBs due to large pores
MCM-22 [25]	Highest concentration of acid sites and high initial activity Less susceptible to deactivation	Catalyst activity is lower due to the fact that cumene can be formed only at the top and bottom of the crystallites. Cumene cannot be diffused into the pores because of a high energy barrier
ZSM-5 [30]	The formation of large byproducts (e.g. DIPBs) is limited due to smaller pores Good resistance to coke build-up	Increased formation of n-propylbenzene High temperatures are necessary to overcome diffusion constraints due to small pore size

Appendix B.3. Selectivity scaling

Selectivity scaling for Beta-zeolites catalyst at 180 °C and propylene conversion of 97.34% used in alkylator [25]:

Cumene and DIPB were assumed to be the only products formed in the alkylation reaction

$$\text{Cumene selectivity} = \frac{90.76}{90.76+8.33} = 91.59\%$$

$$\text{DIPB selectivity} = \frac{8.33}{90.76+8.33} = 8.41\%$$

Pressure conversion [31]

Pressure conversion from kg/cm² to bar:

$$1 \text{ kg/cm}^2 = 98066.5 \text{ Pa}$$

$$1 \text{ bar} = 100\,000 \text{ Pa}$$

$$25 \cdot \frac{98066.5}{100\,000} = 24.52 \text{ bar}$$

Reactor duties calculations

Alkylation reactor (mole flows are taken from material balance table):

$$Q_{cumene} = \dot{n}_{cumene} \cdot \Delta H_{r,cumene} = 119.28 \frac{kmol}{h} \cdot (-99.41) \frac{kJ}{mol} = -1.186 \cdot 10^7 \frac{kJ}{h}$$

$$Q_{DIPB} = \dot{n}_{DIPB} \cdot \Delta H_{r,DIPB} = 12.06 \frac{kmol}{h} \cdot (-100.82) \frac{kJ}{mol} = -1.216 \cdot 10^6 \frac{kJ}{h}$$

$$Q_{total} = Q_{cumene} + Q_{DIPB} = -1.308 \cdot 10^7 \frac{kJ}{h}$$

$$P \text{ (alkylator duty)} = -1.308 \cdot 10^7 \frac{kJ}{h} \cdot \frac{1h}{3600s} = -3.6 \text{ MW}$$

Transalkylation reactor:

$$Q_{cumene} = \frac{\dot{n}_{cumene}}{2} \cdot \Delta H_{r,cumene} = 12.165 \frac{kmol}{h} \cdot 1.14 \frac{kJ}{mol} = 13.87 \cdot 10^3 \frac{kJ}{h}$$

$$P \text{ (transalkylator duty)} = 13.87 \cdot 10^3 \cdot \frac{1h}{3600s} = 3.9 \text{ kW}$$

Appendix B.4. Reactions

Table B.4.1. Reactions involved in cumene production

	Reaction	Type	Reaction Enthalpy, kJ/mol
R1	$C_3H_6 + C_6H_6 \rightarrow C_9H_{12}$	Main	-99
R2	$C_9H_{12} + 2C_3H_6 \rightarrow C_{12}H_{18}$	Side	-101
R3	$C_{12}H_{18} + C_6H_6 \rightarrow 2C_9H_{12}$	Main	2

Appendix B.5. Thermodynamics

Table B.5.1. Physical properties of Propylene, Benzene, Cumene and DIPB

	Propylene		Benzene		Cumene		DIPB	
	From literature	Aspen estimation	From literature	Aspen estimation	From literature	Aspen estimation	From literature	Aspen estimation
State at 25 °C, 1 atm	gas		liquid		liquid		liquid	
Boiling point, K [32, 33]	225.46	225.45	353.24	353.24	425.56	425.56	483.5	483.7
Critical temperature, K [32]	364.90	364.85	562.05	562.05	631	631	674.75 [1]	689
critical pressure (kPa) [32]	4600	4600	4895	4895	3209	3209	2358	2450
Molecular weight, g/mol [33]	42.08		78.11		120.19		162.75	
Freezing point, K [32]	87.9	87.9	278.68	278.68	177.14	177.14	265.05	265.08

ΔH_c^o , kJ/mol [32, 33]	-2057.80 ± 1.10	-1926.2	-3267.62	-3136	-4951.35	-4951	-	5215.44
Critical density, kg/m ³ [33]	228.07 $\pm$ 1.26	227.4	304.64 $\pm$ 0.47	305.1	278.84 $\pm$ 0.96	279.5	278.84 $\pm$ 0.96	271.3
Dynamic viscosity, mPa·s [33, 34]	0.127 - 1.322 for T = 121.8 - 264.7 K	0.080	0.604 – 0.608	0.601	0.611 - 0.690 for T = 303.2 - 313.2 K	0.739	0.179 – 5.546 for T = 233.9 - 504.7 K	0.795
ΔH_{vap}^o , kJ/mol [33]	16.04	14.25	30.5	33.88	45.15	45.27	56.50 $\pm$ 0.30	56.70
Autoignition point, K [32]	770.37	-	864.82	-	698.15	-	722	-
Flash point, K [32]	167.37	-	262.04	-	317.04	-	349	-
ΔH_f^o , kJ/mol [33]	20.41	20.23	Gas: 82.98 Liquid: 49.00 $\pm$ 0.90	82.88	Gas: 3.94 Liquid: -41.20 $\pm$ 1.10	4.00	Gas: -76.51 Liquid: -132.30	-77.6
ΔG_f^o , kJ/mol [32, 33]	62.67	62.64	129.70	129.6	137.10	137.9	148.06	147.8

ΔS_f° kJ/mol·K [33]	, 195.70	-	175.30	-	-449	-	-756	-
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Table B.5.2. Calculated Δ^0H_r , Δ^0G_r , Δ^0S_r

	Reaction 1		Reaction 2		Reaction 3	
Calculations based on	Literature	Aspen Plus V14	Literature	Aspen Plus V14	Literature	Aspen Plus V14
Reaction expression	$C_6H_6 + C_3H_6 \rightarrow C_9H_{12}$		$C_9H_{12} + C_3H_6 \rightarrow C_{12}H_{18}$		$C_{12}H_{18} + C_6H_6 \rightleftharpoons 2C_9H_{12}$	
Δ^0H_r , kJ/mol	-99.41	-99.11	-100.82	-101.83	1.14	2.72
Δ^0G_r , kJ/mol	-55.36	-54.34	-51.80	-52.73	-3.56	-1.61
Δ^0S_r , J/mol·K	-150.43	-144.96	-161.73	-164.47	11.30	14.51

Appendix C. Chapter 3 - Major Equipment Design

Appendix C.1. Heat Exchanger E-102

Heat duty

$$Q = \dot{m}(H_{out} - H_{in}), \tag{C.1.1}$$

where $\dot{m}$ is the cold inlet mixture mass flowrate, kg/s.

$$Q = 24.85 \frac{kg}{s} (898.94 - 598.37) \frac{kJ}{kg} = 7469.16 \frac{kJ}{s}$$

LMTD

$$\Delta T_1 = T_{in, hot} - T_{out, cold} \quad (C.1.2)$$

$$\Delta T_1 = 242.6 - 180 = 62.6 \text{ } ^\circ\text{C}$$

$$\Delta T_2 = T_{out, hot} - T_{in, cold} \quad (C.1.3)$$

$$\Delta T_2 = 242.2 - 27.43945 = 214.76^\circ\text{C}$$

$$\Delta T_{lm} = \frac{\Delta T_2 - \Delta T_1}{\ln \left(\frac{\Delta T_2}{\Delta T_1} \right)} \quad (C.1.4)$$

$$LMTD = \frac{(214.76 - 62.6)^\circ\text{C}}{\ln \frac{214.76}{62.6}} = 123.4^\circ\text{C}$$

Required Heat Transfer Area

Assuming $U = 1200 \text{ W/m}^2\text{K}$:

$$Q = UAF\Delta T_{lm} \quad (C.1.5)$$

Since the hot stream undergoes phase change at nearly constant temperature, the exchanger effectively operates as an ideal counter-current single-pass unit. Consequently, the correction factor is $F = 0.96$.

$$A_{required} = \frac{Q}{FU\Delta T_{lm}} \quad (C.1.6)$$

$$A_{required} = \frac{7469.4 \text{ KW}}{0.96 \times 1200 \frac{\text{W}}{\text{m}^2\text{K}} \times 123.43^\circ\text{C}} = 52.53 \text{ m}^2$$

With 20% margin:

$$A_{design} = A_{required} \cdot 1.2 \quad (C.1.7)$$

$$A_{design} = 52.53 \cdot 1.2 = 63.036 \, m^2$$

Number of Tubes

Area per tube:

$$A_{tube} = \pi d_o L \quad (C.1.8)$$

d_o - outside diameter of tube (m)

L - tube length (m)

$$A_{tube} = 3.1416 \cdot 0.019 \, m \cdot 4.9 \, m = 0.292 \, m^2$$

$$N_t = \frac{A_{design}}{A_{tube}} \quad (C.1.9)$$

$$N_t = \frac{63.036 \, m^2}{0.292 \, m^2} = 215.7 \rightarrow 215 \, tubes$$

Shell-Side Heat Transfer Coefficient

Reynolds number is calculated by:

$$Re = \frac{G_s d_e}{\mu_s}, \quad (C.1.10)$$

where G_s is the mass velocity, kg/m².

$$G_s = \frac{\dot{m}}{A_s} \quad (C.1.11)$$

$$A_s (\text{cross flow area}) = \frac{P_t - D_{o, tube}}{P_t} \cdot D_s \cdot L_{buffle} \quad (\text{C.1.12})$$

$$D_e = \frac{1.10 \cdot (P_t^2 - 0.917 D_o^2)}{D_o^2} \quad (\text{C.1.13})$$

μ – Viscosity, $Pa \times s$

Summing those formulae give the final expression for Re:

$$Re = \frac{1551.27 \frac{kg}{m^2} \cdot 0.01349 m}{0.000276 Pa \cdot s} = 75812.36$$

Calculation of Prandtl number:

$$Pr = \frac{C_p \cdot \mu}{k} \quad (\text{C.1.14})$$

$$Pr = \frac{2017.4 \frac{J}{kg \cdot K} \cdot 0.000276 Cp}{0.1148 \frac{W}{m \cdot K}} = 4.84876$$

From Figure C.1.3: $j_h = 0.0025$ approximately.

Colburn j-factor formula to calculate h_s :

$$h_s = j_h \cdot Re \cdot \frac{k}{D_e} \cdot Pr^{\frac{1}{3}} \quad (\text{C.1.15})$$

k - Conductivity of cold side mixture ($W/m \cdot K$)

$$h_s = 0.0025 \cdot 75812.36 \cdot \frac{0.1148 \frac{W}{m \cdot K}}{0.01349 m} \cdot 4.84876^{\frac{1}{3}} = 2731.09 \frac{W}{m^2 K}$$

Tube-Side Heat Transfer Coefficient

Using the same Colburn j-factor correlation (Equation C.1.15):

$$h_i = j_h \cdot Re \cdot \frac{k}{D_e} \cdot Pr^{\frac{1}{3}} = 0.055 \cdot 77997.15 \cdot \frac{0.04579 \frac{W}{m \cdot K}}{0.0173 m} \cdot 0.92278^{\frac{1}{3}} = 11058.05 \frac{W}{m^2 K}$$

Overall Heat Transfer Coefficient

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_{od}} + \frac{d_o \ln\left(\frac{d_o}{d_i}\right)}{2k_w} + \frac{d_o}{d_i} \frac{1}{h_{id}} + \frac{d_o}{d_i} \frac{1}{h_i} \quad (C.1.16)$$

$$U_o = 1257 \frac{W}{m^2 K}$$

The obtained value is for U_o with fouling. To get the value of clean U_o without fouling, the units with fouling factors are eliminated from the formula:

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{d_o \ln\left(\frac{d_o}{d_i}\right)}{2k_w} + \frac{d_o}{d_i} \frac{1}{h_i} \quad (C.1.17)$$

$$U_o = 2060 \frac{W}{m^2 K}$$

k_w - thermal conductivity of tube wall

h_{id} - inside fouling coefficient

h_{od} - outside fouling coefficient

Tube-Side Pressure Drop

$$\Delta P_t = \left(8j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-0.14} + 2.5 \right) \frac{\rho_u^2}{2} \quad (C.1.18)$$

$$\Delta P_t = \left(8 \cdot 0.0035 \cdot 283.23 \cdot \left(\frac{0.01804}{0.37} \right)^{-0.14} + 2.5 \right) \cdot \frac{16.9815 \frac{m}{s^2} \cdot 4.7889^2 \frac{m^2}{s^2}}{2}$$

$$= 2844.069 \frac{N}{m^2}$$

j_f - tube side friction factor (Figure C.1.1)

μ - viscosity of tube side fluid

μ_w - viscosity of water

ρ - mass density of tube side fluid

ϑ - linear velocity of the fluid flow

Converting to bars:

$$\Delta P_t = 0.028441 \text{ bar}$$

Shell-Side Pressure Drop

$$\Delta P_s = 8j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_B} \right) \frac{\rho_s u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14} \quad (C.1.19)$$

j_f - Shell-side friction factor (Figure B4)

D_s - Shell diameter

d_e - Equivalent diameter

l_B - Baffle spacing

$$\Delta P_s = 8 \cdot 0.0035 \cdot \left(\frac{447.48}{13.49} \right) \cdot \left(\frac{4.9}{0.179} \right) \frac{739.599 \frac{kg}{m^3} \times 2.0975^2 \frac{m^2}{s^2}}{2} \cdot \left(\frac{0.276}{0.37} \right)^{-0.14}$$

$$= 43093.34 \frac{N}{m^2}$$

$$\Delta P_s = 0.431 \text{ bars}$$

Number of baffles

$$N_B = \frac{L}{l_b} - 1 \quad (\text{C.1.20})$$

$$N_B = \frac{4.9 \text{ m}}{0.179 \text{ m}} - 1 = 26$$

Shell Thickness

$$t = \frac{PR}{SE - 0.6P} \quad (\text{C.1.21})$$

P - design pressure, MPa

R - inside radius of shell, m

S - Allowable Stress of Material, MPa

E - Weld Joint Efficiency

$$t_{total} = t + CA \quad (\text{C.1.22})$$

$$t_{total} = \frac{3.5 \text{ MPa} \cdot 223.75 \text{ mm}}{130 \text{ MPa} \cdot 0.85 - 0.6 \cdot 3.5} + 1.5 = 8.72 \text{ mm}$$

Typical corrosion allowance for steam service: 1.5 mm

Shell outer diameter

$$D_{OD} = D_{ID} + 2 \cdot t \quad (\text{C.1.23})$$

$$D_{OD} = 447.48 \text{ mm} + 2 \cdot 8.72 \text{ mm} = 464.92 \text{ mm}$$

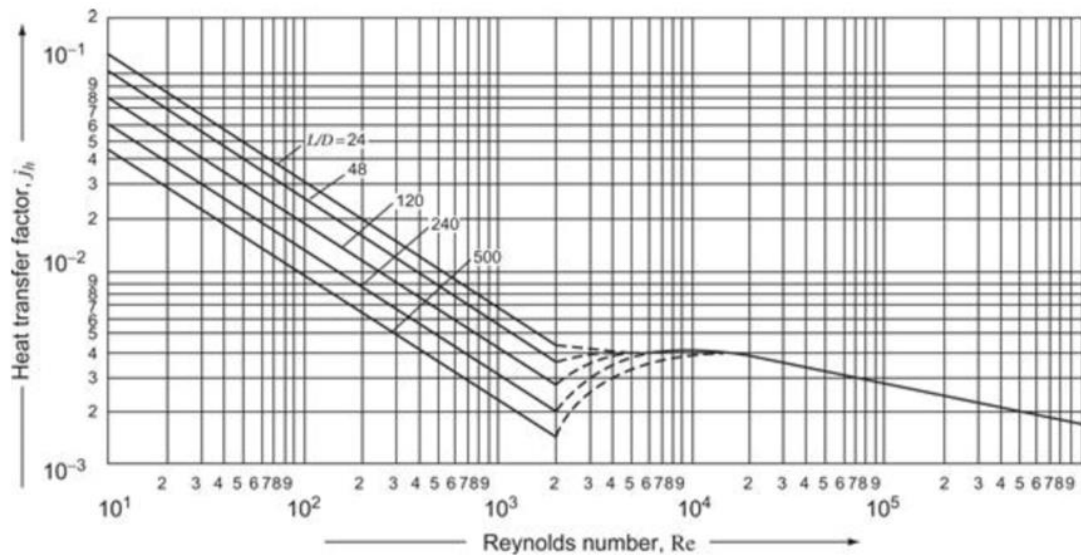


Figure C.1.1. Tube-side Friction factor

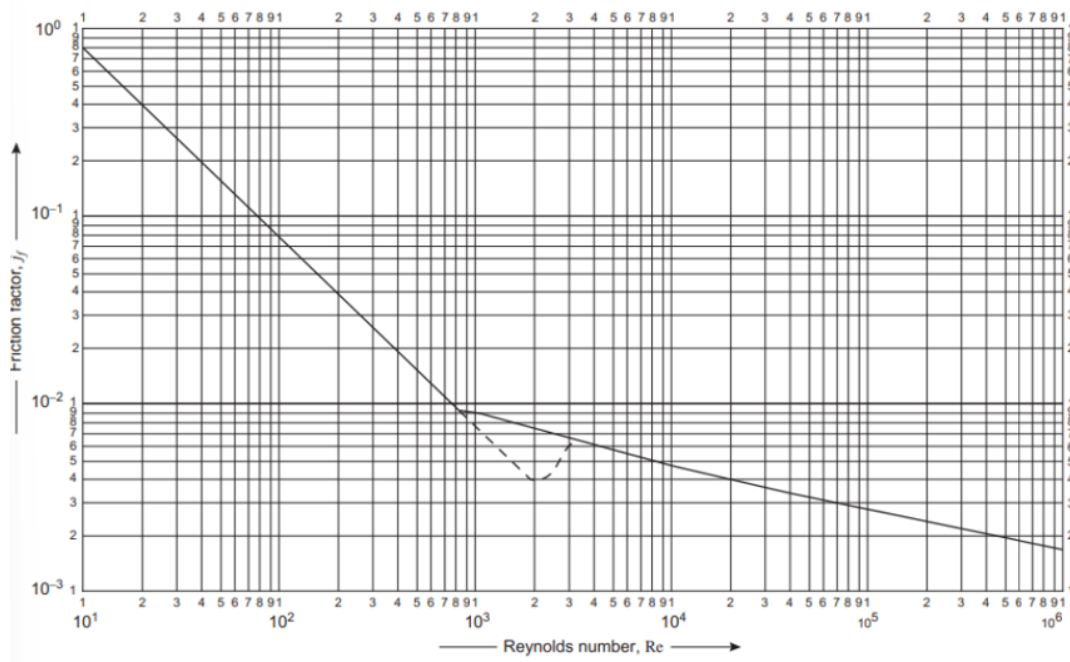


Figure C.1.2. Tube-side Friction factor

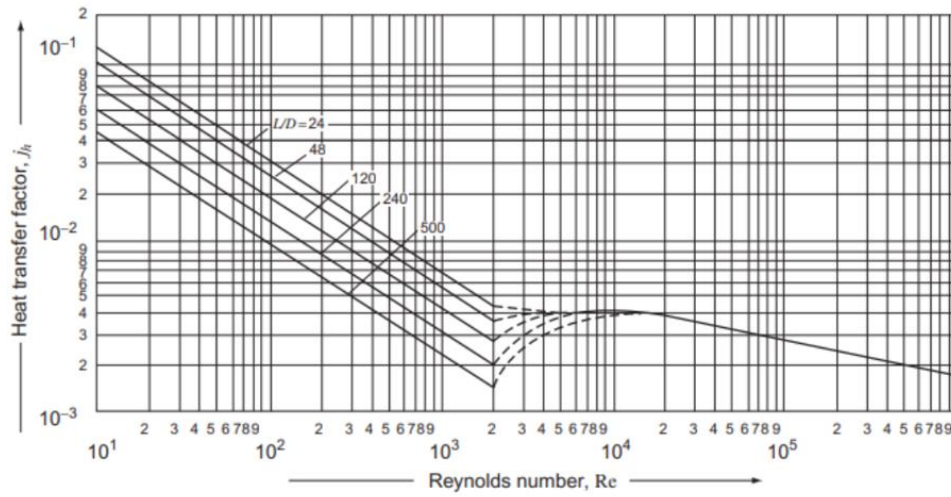


Figure C.1.3. Shell-side Heat transfer factor

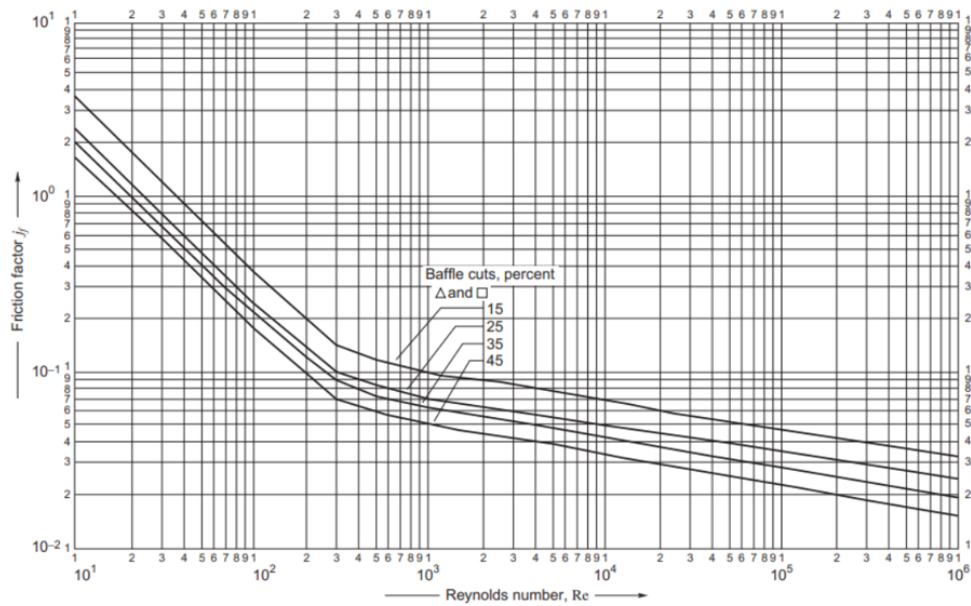


Figure C.1.4. Shell-side Friction factor

Appendix C.2. Reactors R-101 and R-102

Dimensions of the reactors

The working volume of R-101 was calculated by solving the following system of ODEs in Python (solve_ivp from SciPy):

$$\frac{dF_P}{dV} = -(r_1 + r_2) \quad (\text{C.2.1})$$

$$\frac{dF_B}{dV} = -r_1 \quad (\text{C.2.2})$$

$$\frac{dF_C}{dV} = r_1 - r_2 \quad (\text{C.2.3})$$

$$\frac{dF_D}{dV} = r_2 \quad (\text{C.2.4})$$

$$\frac{dT}{dV} = -\frac{\Delta H_1(T)r_1 + \Delta H_2(T)r_2}{F_{total}c_{p,mix}(T)} \quad (\text{C.2.5})$$

In equations C.2.1-C.2.5, F_{total} is the total mole flow of the components (mol/s), ΔH_1 and ΔH_2 are the enthalpies for r_1 and r_2 , respectively (J/mol), $C_{p,mix}$ is the heat capacity of the mixture (J/mol·K). As a result, $V_{catalyst} = 7.21 \text{ m}^3$.

The volume of the reactor bed is calculated by:

$$V_{total} = \frac{V_{catalyst}}{1 - \varepsilon} = \frac{7.21 \text{ m}^3}{0.5} = 14.42 \text{ m}^3 \quad (\text{C.2.6})$$

where ε is the bed voidage.

For the reversible transalkylation reaction in R-102, the reaction rate is expressed as:

$$r = r_f - r_b = k_f x_B x_D - k_b x_C^2$$

The required volume for the reactor R-102 was calculated by solving the following system of ODEs in Python:

$$\frac{dF_D}{dV} = -r \quad (\text{C.2.7})$$

$$\frac{dF_B}{dV} = -r \quad (\text{C.2.8})$$

$$\frac{dF_C}{dV} = 2r \quad (\text{C.2.9})$$

$$\frac{dT}{dV} = \frac{-\Delta H_r \cdot r}{F_T C_{p,mix} + (1-\varepsilon)C_{p,s}} \quad (\text{C.2.10})$$

Where, H_r is the heat of reaction at temperature T in kJ/kmol, $C_{p, \text{mix}}$ is the heat capacity of a mixture, kJ/kmol·K, $C_{p, \text{mix}}$ is the heat capacity of the solid catalyst, kJ/kmol·K, F_T is the total flowrate, kmol/hr.

The volume of the transalkylator is calculated by:

$$V = \frac{F_T MW_{mix}}{\rho_{liq}} \quad (\text{C.2.11})$$

Heat of reaction

The enthalpy is a function of temperature; thus, the overall heat of reaction differs at higher reactor temperatures. The following equation from the Peng-Robinson EOS calculates the heat of reaction:

$$H(T) = H^{ig} + \Delta H_{dep} \quad (\text{C.2.12})$$

Table C.2.1. Enthalpy values of each compound

	H^{ig} , kJ/kmol	$\Delta H_{dep, \text{avg}}$, kJ/kmol	H , kJ/kmol
Benzene	49	-24.00	25.0
Propene	20.23	-54.45	-34.22
Cumene	-24	-33.92	-57.92
DIPB	-78	-41.72	-119.72

$$H_1 = (-57.92) - (25) - (-34.22) = -48.7 \frac{\text{kJ}}{\text{mol}}$$

$$H_2 = (-119.72) - (-57.92) - (25) = -86.8 \frac{\text{kJ}}{\text{mol}}$$

Table C.2.2. Final enthalpy values at R-102 temperature conditions

	H_{ig} , kJ/kmol	ΔH_{dep} at T=240 °C, kJ/kmol	ΔH_{dep} at T=255 °C, kJ/kmol	$\Delta H_{dep, avg}$, kJ/kmol	H, kJ/kmol
Benzene	49	-21.96	-19.96	-20.96	28.04
Cumene	-24	-32.39	-31.41	-31.9	-55.90
DIPB	-78	-40.28	-39.38	-39.83	-117.83

$$H = 2 \cdot (-55.90) - (-117.83 + 28.04) = -22.01 \text{ kJ/kmol}$$

The number of tubes in the reactors was calculated by:

$$V_{tube} = \frac{1}{4} \pi d_{in}^2 L = \frac{1}{4} \pi (50.8 \times 10^{-3} \text{ m})^2 (6 \text{ m}) = 0.0122 \text{ m}^3 \quad (\text{C.2.13})$$

$$N_{tubes} = \frac{V_{bed}}{V_{tube}} = \frac{14.96 \text{ m}^3}{0.0122 \text{ m}^3} = 1230 \text{ tubes in } R - 101 \quad (\text{C.2.14})$$

$$N_{tubes} = \frac{V_{bed}}{V_{tube}} = \frac{6.69 \text{ m}^3}{0.0122 \text{ m}^3} = 551 \text{ tubes in } R - 102$$

Here, d_{in} is the inner diameter of the tube (m) and L is the length of the tube (m).

Pressure drop

The pressure drop within the reactors is estimated using the Ergun equation [35]:

$$\frac{\Delta P}{L} = \frac{150u_0\mu}{(\phi_s d_p)^2} \frac{(1-\varepsilon)^2}{\varepsilon^3} + \frac{1.75\rho u_0^2}{\phi_s d_p} \left(\frac{1-\varepsilon}{\varepsilon^3} \right) \quad (C.2.15)$$

Here, μ is the dynamic viscosity of the mixture (Pa s), ϕ_s is the shape factor, d_p is the diameter of the particle (m), and ρ is the density of the mixture (kg/m³). Superficial velocity, u_0 , in R-101 is:

$$\begin{aligned} u_0 &= \frac{Q_{tube}}{A_{tube}} = \frac{Q_{tube}}{\frac{1}{4}\pi d_{in}^2} = \frac{\frac{0.0386 \text{ m}^3/\text{s}}{1230 \text{ tubes}}}{\frac{1}{4}\pi(50.8 \times 10^{-3} \text{ m})^2} \\ &= 0.0155 \frac{\text{m}}{\text{s}} \end{aligned} \quad (C.2.16)$$

Meanwhile, in R-102:

$$u_0 = \frac{Q_{tube}}{A_{tube}} = \frac{Q_{tube}}{\frac{1}{4}\pi d_{in}^2} = \frac{\frac{0.0047 \text{ m}^3/\text{s}}{551 \text{ tubes}}}{\frac{1}{4}\pi(50.8 \times 10^{-3} \text{ m})^2} = 0.0042 \frac{\text{m}}{\text{s}}$$

Q_{tube} and A_{tube} are the volumetric flow rate (m³/s) and cross-sectional area (m²) of one tube.

Actual velocity can be determined using the following:

$$u_{actual} = \frac{u_0}{\varepsilon} = \frac{0.0155 \frac{\text{m}}{\text{s}}}{0.5} = 0.031 \frac{\text{m}}{\text{s}} \text{ in } R - 101 \quad (C.2.17)$$

$$u_{actual} = \frac{u_0}{\varepsilon} = \frac{0.0042 \frac{\text{m}}{\text{s}}}{0.5} = 0.0084 \frac{\text{m}}{\text{s}} \text{ in } R - 102$$

Other parameter values used in the calculation of pressure drop are taken directly from Aspen Plus V14 simulation: $\mu = 1.012 \cdot 10^{-4}$ Pa s, $\rho = 644.3$ kg/m³ for the feed in R-101 and $\mu = 8.892 \cdot 10^{-5}$ Pa s, $\rho = 591.8$ kg/m³ in R-102.

From this, the resulting pressure drops are 0.0395 bar for R-101 and 0.0038 bar for R-102.

Wall thickness

Wall thickness is characterized by ASME table for maximum allowable stress:

$$t = \frac{Pd_{out}}{2(SE - PY)} + c \quad (C.2.18)$$

$$t_{required} = \frac{t}{\text{mill tolerance}} \quad (C.2.19)$$

In Equation C.2.12, c is the corrosion allowance, d_{out} is the outer diameter of the tube, E is the quality factor, P is the design pressure, S is the allowable stress, and Y is a coefficient that depends on the type of material. This way, the R-101 and R-102 wall thicknesses resulted in 2.72 mm and 2.43 mm, respectively.

Table C.2.3. Parameters for thickness calculations

	R – 101	R – 102
P, bar	38.5	26.95
D, mm	60.3	
S, bar	1299.77	1272.08
E	1	
W	1	
Y	0.4	
c	1.5	
Mill tolerance	$1 - 0.125 = 0.875$	

$$t_{R-101} = \frac{38.5 \text{ bar} \cdot 60.3 \text{ mm}}{2(1299.77 \text{ bar} + 38.5 \text{ bar} \cdot 0.4)} + 1.5 = 2.38 \text{ mm}$$

$$t_{req, R-101} = \frac{2.38}{0.875} = 2.72 \text{ mm}$$

$$t_{R-102} = \frac{26.95 \text{ bar} \cdot 60.3 \text{ mm}}{2(1272.08 \text{ bar} + 26.95 \text{ bar} \cdot 0.4)} + 1.5 = 2.13 \text{ mm}$$

$$t_{req, R-102} = \frac{2.13}{0.875} = 2.43 \text{ mm}$$

Appendix C.3. Distillation columns T-101, T-102, T-103

$$\ln p_i^{sat} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{6i}T^{C_{7i}}; C_{8i} \leq T \leq C_{9i} \quad (\text{C.3.1})$$

Table C.3.1. Extended Antoine's equation parameters (Retrieved from Aspen)

Components	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈	C ₉
BENZENE	71,5941	-6486,2	0	0	-9,21940	6,98440E-06	2	278,68	562,05
PROPENE	32,3921	-3097,8	0	0	-3,44250	9,99890E-17	6	87,89	364,85
PROPANE	47,5651	-3492,6	0	0	-6,06690	1,09190E-05	2	85,47	369,83
CUMENE	91,2971	-8674,6	0	0	-11,9220	7,00480E-06	2	177,14	631,00
DIPB	65,1041	-9057,0	0	0	-7,50330	2,57090E-18	6	256,08	689,00

Entrainment values were estimated from Figure C.3.1:

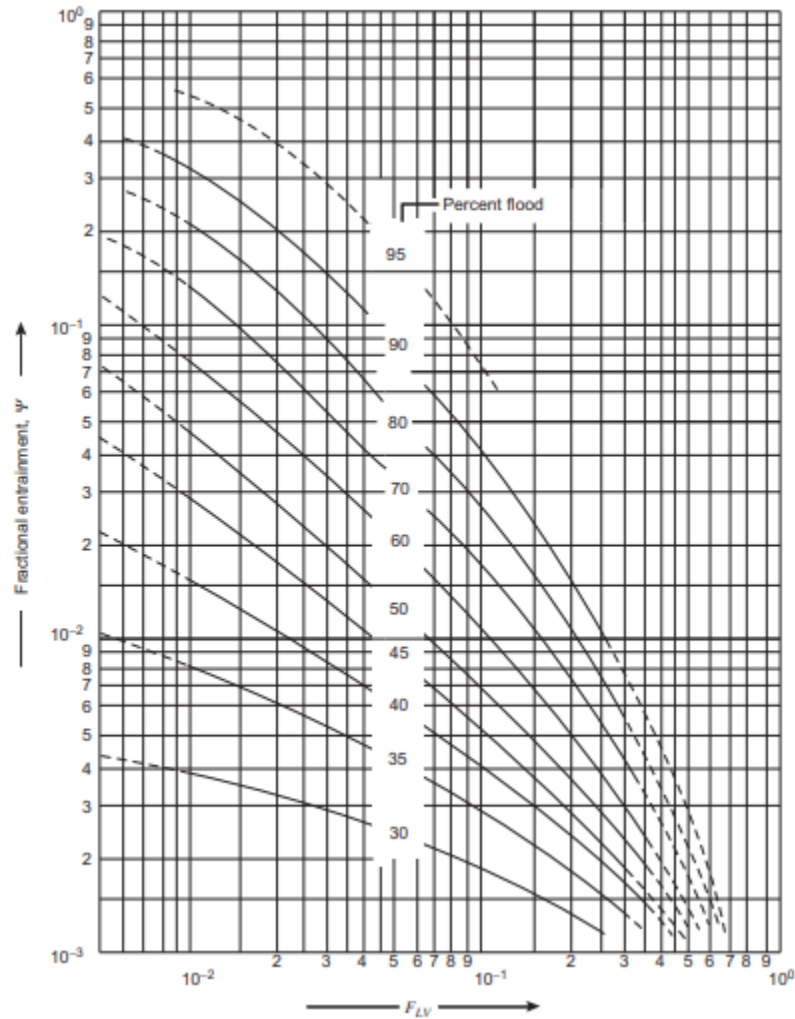


Figure C.3.1. Entrainment correlation from sieve plates.

To use this correlation, the following additional parameters were calculated: liquid-vapor flow factor, F_{LV} , and percentage flood.

The liquid-vapor flow factor was calculated by the equation below:

$$F_{LV} = \frac{L_w}{V_w} \sqrt{\frac{\rho_v}{\rho_L}} \quad (\text{C.3.2})$$

Where,

L_w – liquid mass flow rate, kg/s

V_w – vapor mass flow rate, kg/s

ρ_v – density of vapor, kg/m³

ρ_L – density of liquid, kg/m³

Percentage flooding was calculated by the equation below:

$$percentage\ flood = \frac{u_n}{u_f} \quad (C.3.3)$$

Where,

u_n – actual velocity based on net area

u_f – flooding vapor velocity

Flooding velocity is calculated from the equation below:

$$u_f = K1 \sqrt{\frac{\rho_L - \rho_v}{\rho_v}} \quad (C.3.4)$$

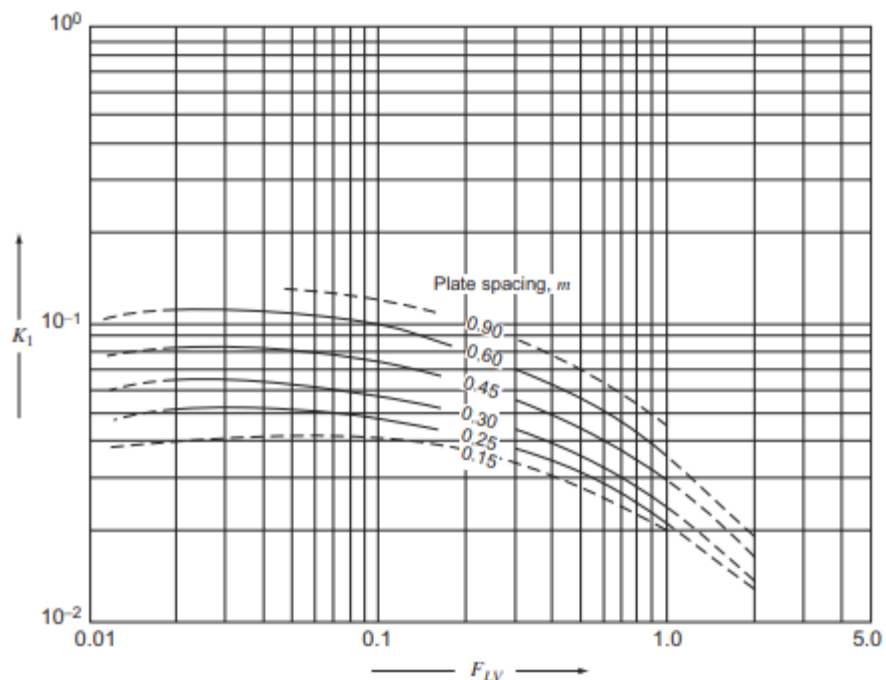


Figure C.3.2. Flooding velocity for sieve plates.

K_1 is needed to be additionally corrected by the following values:

Table C.3.2. Corrections of K_1 values

Hole: active area ratio	Multiply K_1 by
0.10	1.0
0.08	0.9
0.06	0.8

Procedure of Murphree efficiency estimation

First, hydraulic data were obtained from RadFrac, simulated from the calculated number of stages and the reflux ratio calculated by DSTWU. Then, in order to use Figure C.3.1, the F_{LV} factor was estimated from the hydraulics data.

Column T-101 supplementary data:

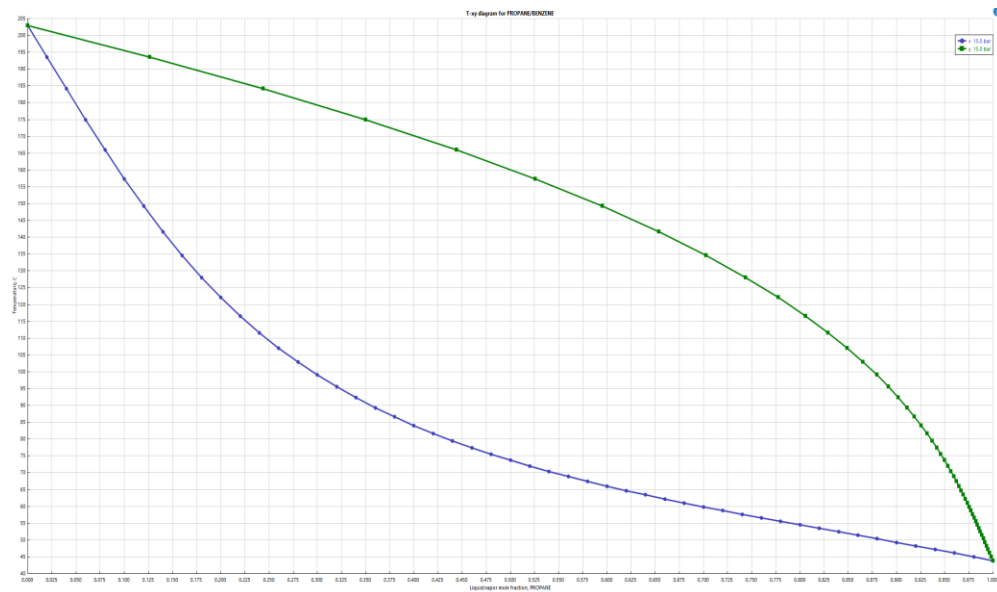


Figure C.3.3. T-xy diagram of propane/benzene at 15 bar from Aspen Plus v14

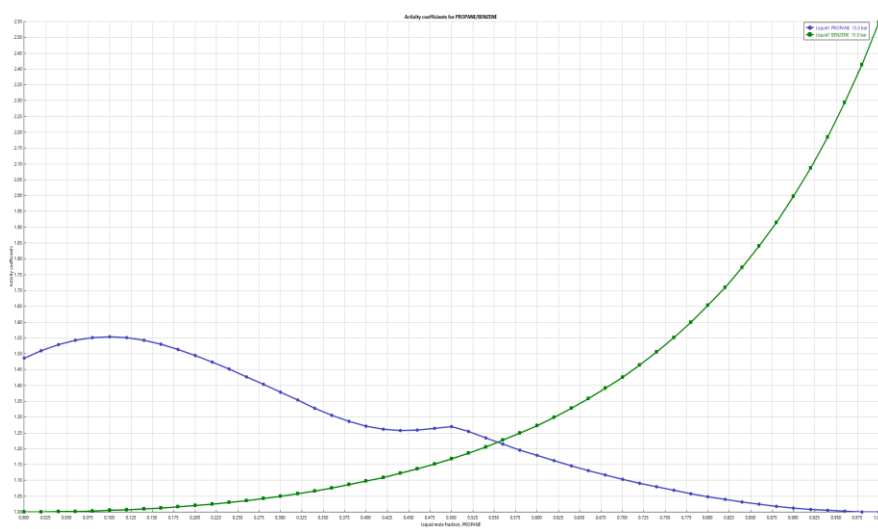


Figure C.3.4. Activity coefficients for propane/benzene of T-101 column from Aspen Plus v14

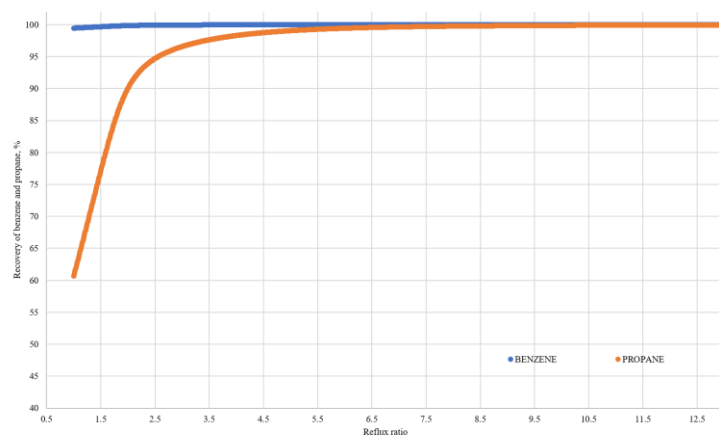


Figure C.3.5. Benzene and propane recovery vs. reflux ratio for T-101 column

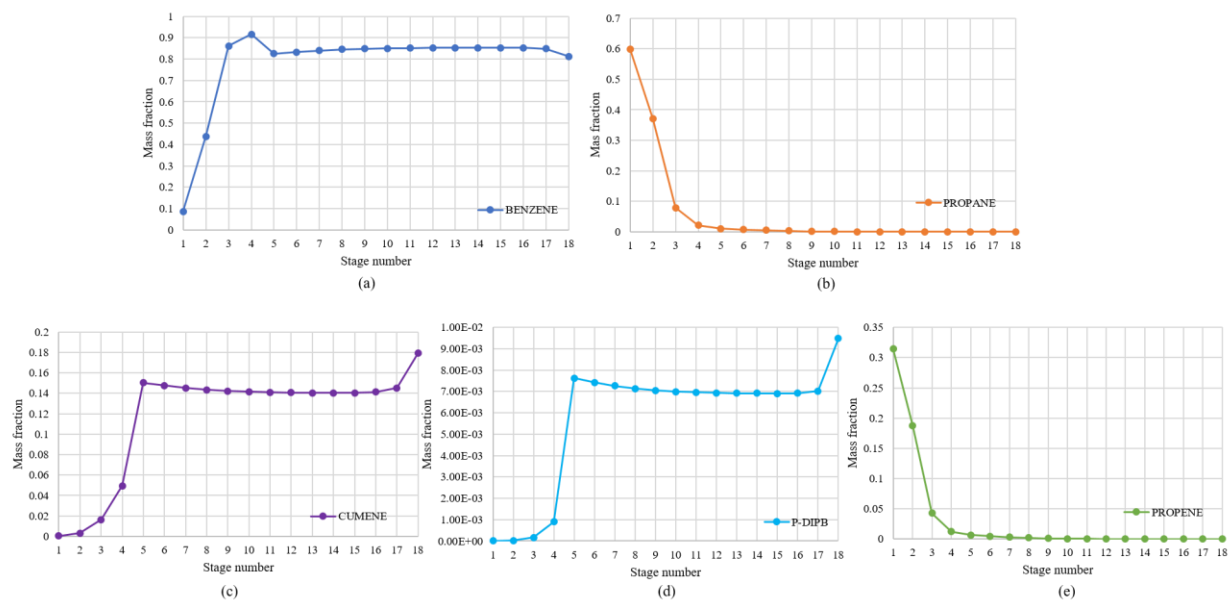


Figure C.3.6. Composition vs Stage for T-101 column for a) benzene; b) propane; c) cumene; d) p-DIPB, and e) propene

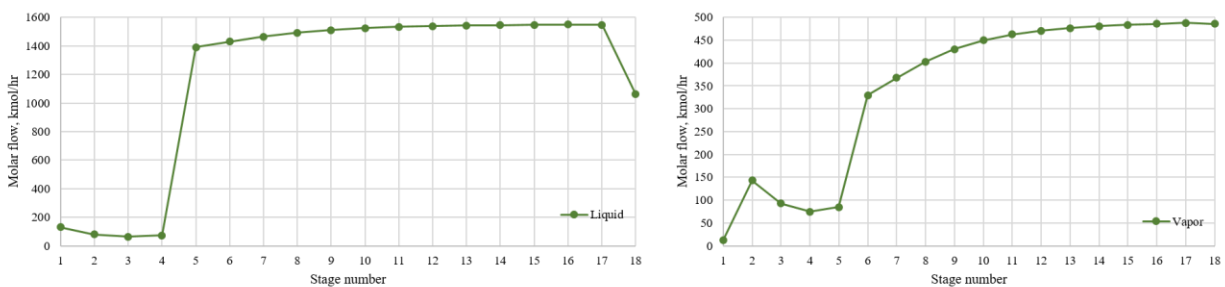


Figure C.3.7. Temperature ($^{\circ}\text{C}$) vs Stage number

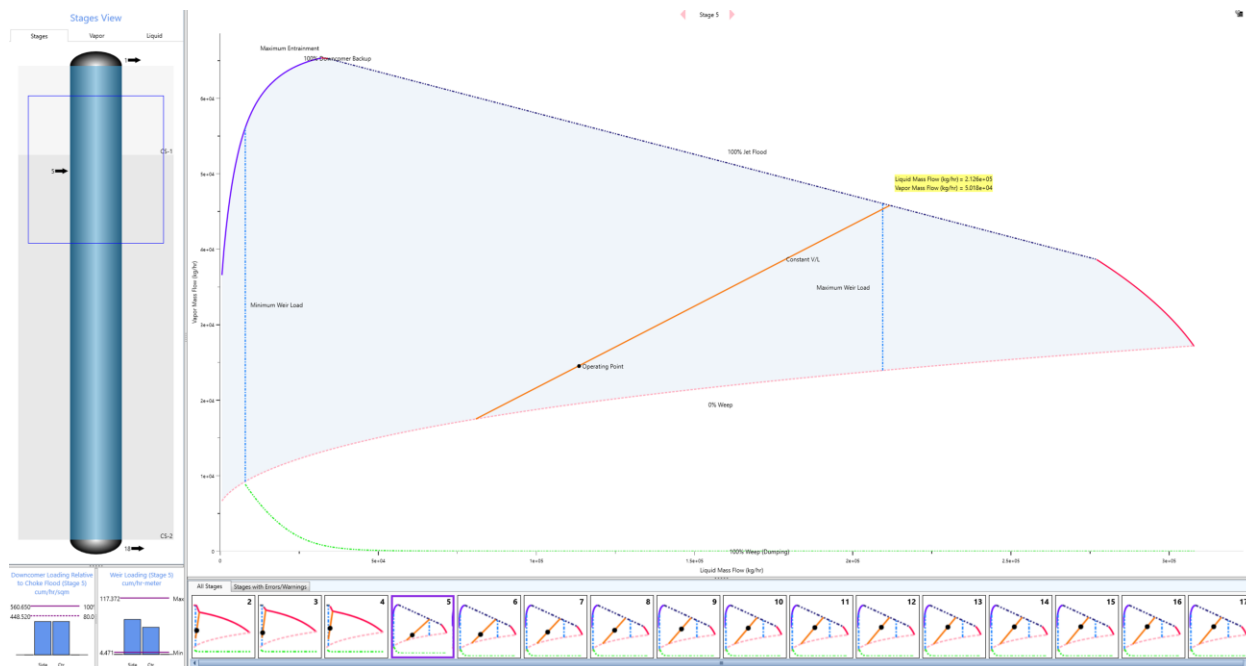


Figure C.3.8. Hydraulic plot of T-101 column

Specifications	Calculation Options	Convergence	Comments
Column specifications ☒ Number of stages: 16 ☐ Reflux ratio:	Pressure Condenser: 14.85 bar Reboiler: 15.5 bar		
Key component recoveries Light key Comp: PROPANE Recov: 0.999 Heavy key Comp: BENZENE Recov: 0.0001	Condenser specifications ☐ Total condenser ☒ Partial condenser with all vapor distillate ☐ Partial condenser with vapor and liquid distillate Distillate vapor fraction: 1		

Figure C.3.9. Input of DSTWU

Configuration	Streams	Pressure	Condenser	Reboiler	3-Phase	Comments
Setup options Calculation type: Equilibrium Number of stages: 18 Stage Wizard Condenser: Partial-Vapor Reboiler: Kettle Valid phases: Vapor-Liquid Convergence: Standard						
Operating specifications Distillate rate: Mole 12.0705 kmol/hr Reflux ratio: Mole 10.863 Free water reflux ratio: 0 Feed Basis Design and specify column internals						

Figure C.3.10. Input of RadFrac for T-101 column

Column T-102 supplementary data:

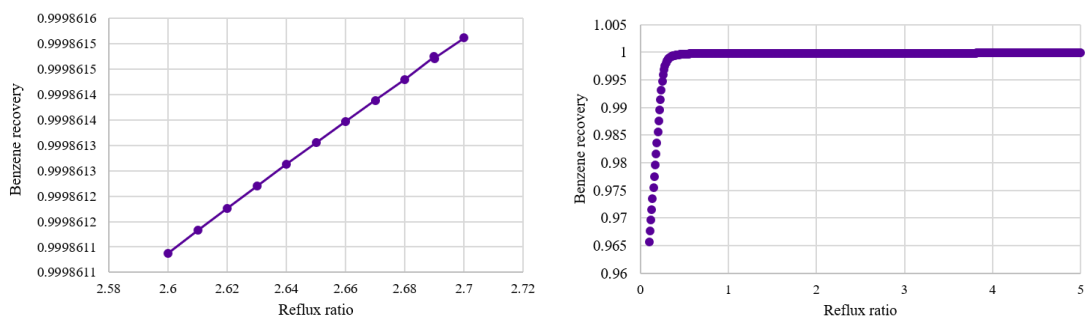


Figure C.3.11. Benzene recovery vs. reflux ratio for T-102 column

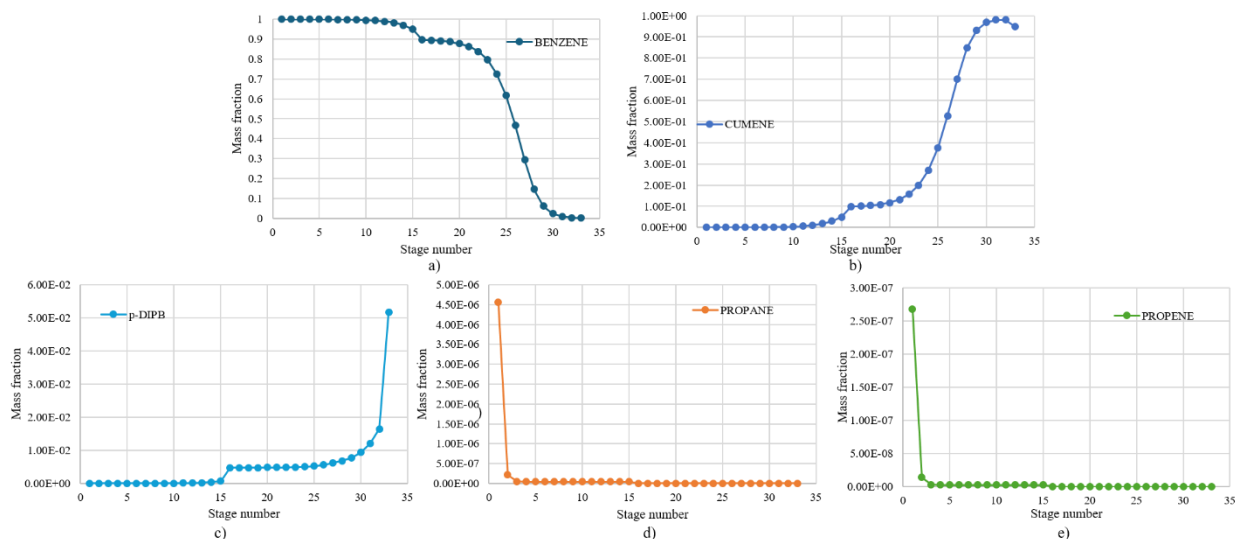


Figure C.3.12. Composition vs Stage for T-102 column for a) benzene; b) cumene; c) p-DIPB; d) propane, and e) propene

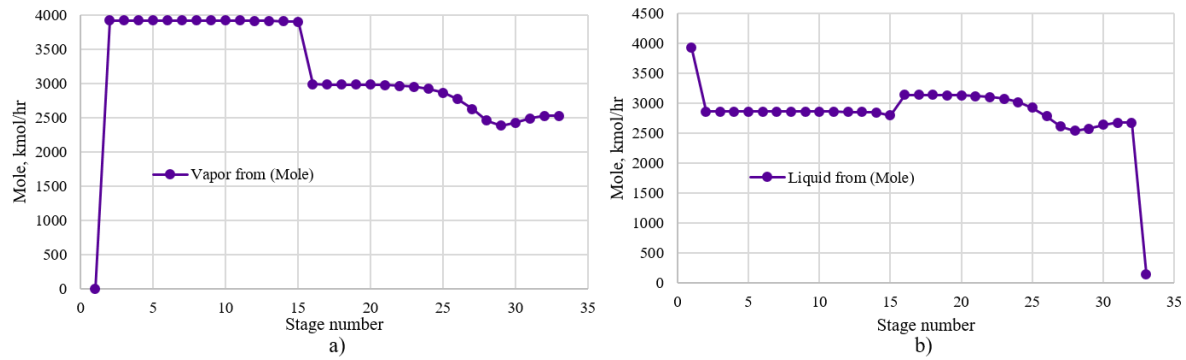


Figure C.3.13. Mole flows vs Stage a) vapor from and b) liquid from for T-102 column

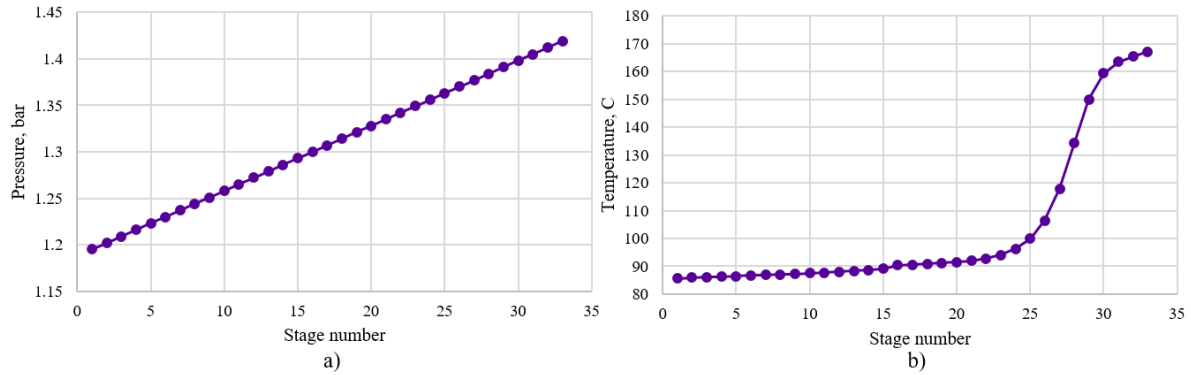


Figure C.3.14. Operating conditions vs stage a) pressure, bar and b) temperature, °C

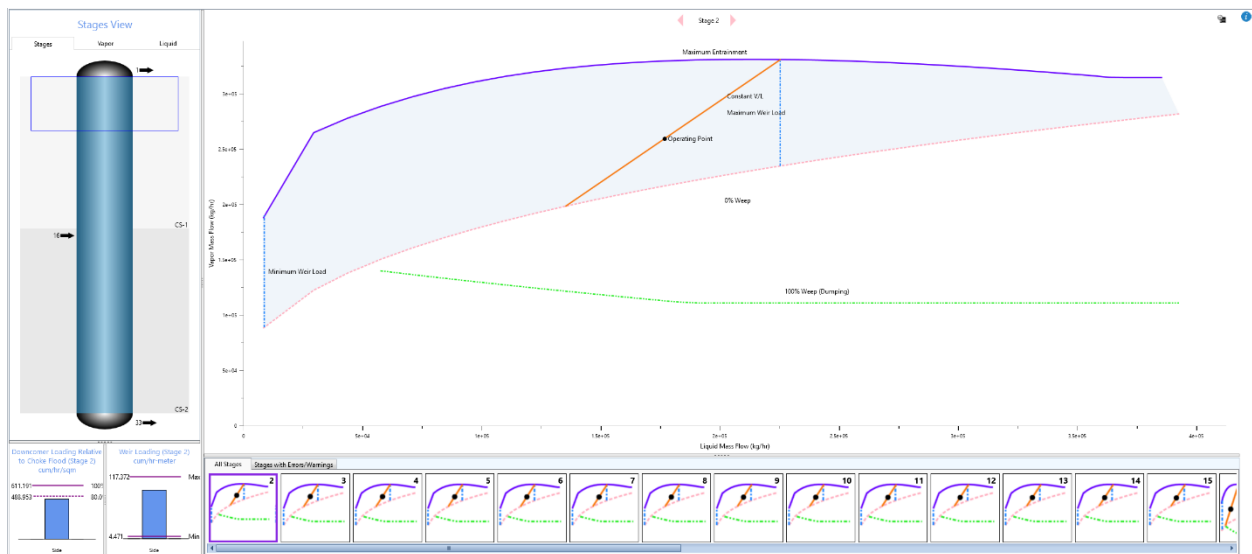


Figure C.3.15. Hydraulic plot of T-102 column

Setup options

Calculation type: *Equilibrium*

Number of stages: *33* Stage Wizard

Condenser: *Total*

Reboiler: *Kettle*

Valid phases: *Vapor-Liquid*

Convergence: *Standard*

Operating specifications

Distillate rate: *Mole* *1062.42* *kmol/hr*

Reflux ratio: *Mole* *2.6899*

Free water reflux ratio: *0* Feed Basis

Design and specify column internals

Figure C.3.16. Input to RadFrac T-102

Column specifications

☒ Number of stages: *23*

☐ Reflux ratio:

Pressure

Condenser: *1.195* *bar*

Reboiler: *1.419* *bar*

Key component recoveries

Light key

Comp: *BENZENE*

Recov: *0.999867*

Heavy key

Comp: *CUMENE*

Recov: *0.0001*

Condenser specifications

☒ Total condenser

☐ Partial condenser with all vapor distillate

☐ Partial condenser with vapor and liquid distillate

Distillate vapor fraction: *0*

Figure C.3.17. Input to DSTWU T-102

Column T-103 supplementary data:

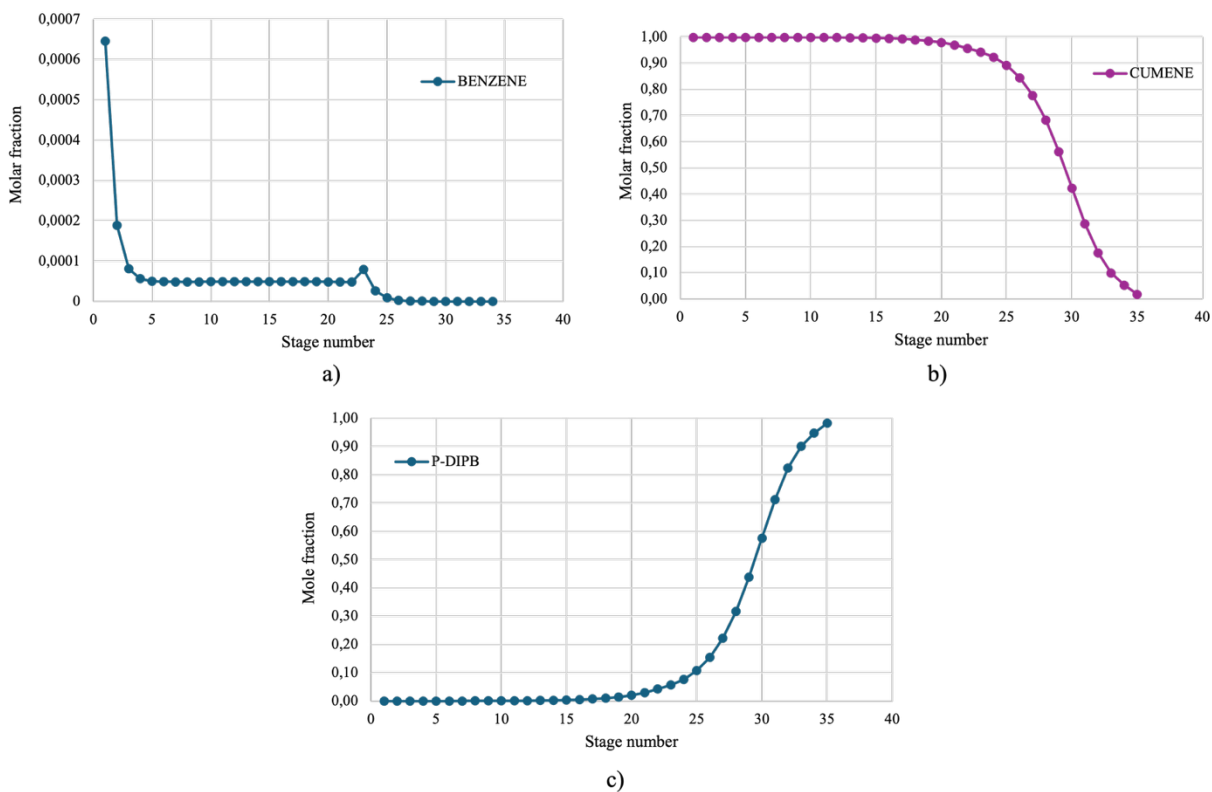


Figure C.3.18. Composition vs Stage for T-103 column for a) benzene; b) cumene; c) P-DIPB

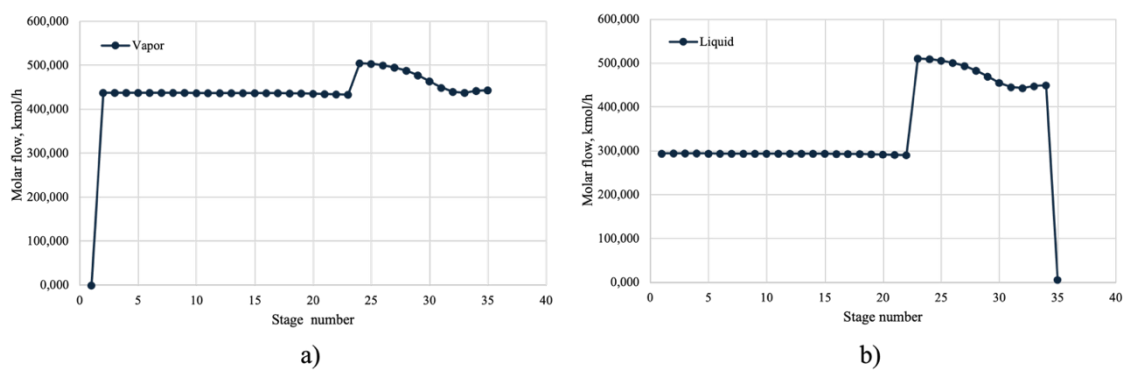


Figure C.3.19. Mole flows vs Stage a) vapor from and b) liquid from for T-102 column

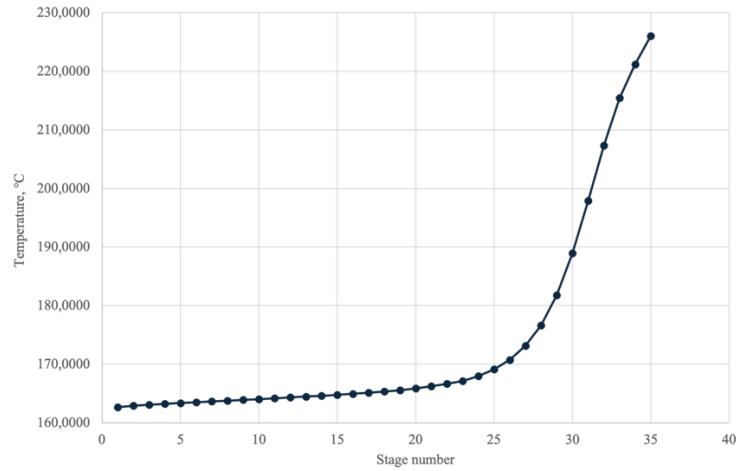


Figure C.3.20. Temperature (°C) vs stages plot

Setup options

Calculation type

Equilibrium

Number of stages

35

Stage Wizard

Condenser

Total

Reboiler

Kettle

Valid phases

Vapor-Liquid

Convergence

Standard

Operating specifications

Distillate rate

Mole

142.998

kmol/hr

Reflux ratio

Mole

2.06

Free water reflux ratio

0

Feed Basis

Design and specify column internals

Figure C.3.21. T-103 RadFrac input

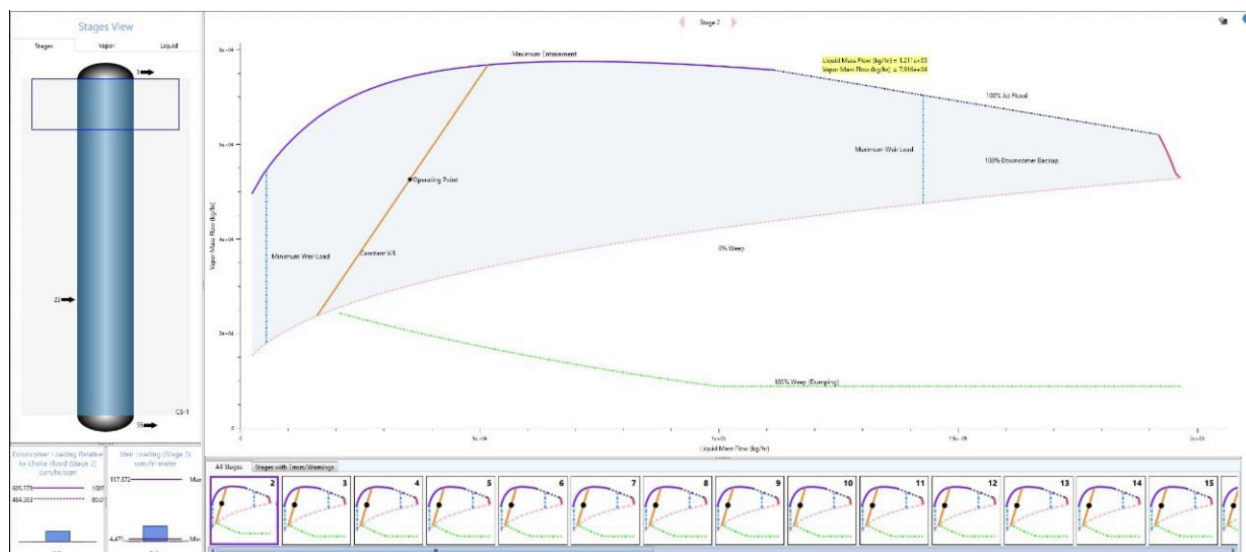


Figure C.3.22. Hydraulic plot of T-103 column

Condenser / Top stage performance			
	Name	Value	Units
>	Temperature	435.841	K
>	Subcooled temperature		
>	Heat duty	-4423.48	kW
>	Subcooled duty		
>	Distillate rate	142.998	kmol/hr
>	Reflux rate	294.576	kmol/hr
>	Reflux ratio	2.06	
>	Free water distillate rate		
>	Free water reflux ratio		
>	Distillate to feed ratio		

Reboiler / Bottom stage performance			
	Name	Value	Units
>	Temperature	499.213	K
>	Heat duty	5159.86	kW
>	Bottoms rate	5.92059	kmol/hr
>	Boilup rate	443.817	kmol/hr
>	Boilup ratio	74.9618	
>	Bottoms to feed ratio		

Figure C.3.23. T-103 RadFrac simulation results

Column specifications

☒ Number of stages

☐ Reflux ratio

Key component recoveries

Light key

Comp

Recov

Heavy key

Comp

Recov

Pressure

Condenser

Reboiler

Condenser specifications

☒ Total condenser
 ☐ Partial condenser with all vapor distillate
 ☐ Partial condenser with vapor and liquid distillate

Distillate vapor fraction

Figure C.3.24. T-103 DSTWU input

▶	Minimum reflux ratio	0.413128	
▶	Actual reflux ratio	0.541062	
▶	Minimum number of stages	14.0094	
▶	Number of actual stages	31	
▶	Feed stage	19.4869	
▶	Number of actual stages above feed	18.4869	
▶	Reboiler heat duty	2988.69	kW
▶	Condenser heat duty	-2252.3	kW
▶	Distillate temperature	435.841	K
▶	Bottom temperature	499.232	K
▶	Distillate to feed fraction	0.960244	
▶	HETP		

Figure C.3.25. T-103 DSTWU simulation results

Appendix D. Estimation of utility prices

To estimation of the price of the electricity and, similarly, of high-pressure steam, were based on the following assumptions for Atyrau in 2026:

- Natural gas price: 36.4 KZT/m³ [36]
- Boiler efficiency: 90% [37,38]
- Exchange rate: 500 KZT/USD [39, 40]

Assuming 20 °C temperature drop:

$$q = cp\Delta T = 2.7 * 20 = 54 \text{ kg/h}$$

$$m_{steam} = \frac{3600}{54} = 66.7 \text{ kg}$$

$$Q_{fuel} = \frac{3600}{0.9} = 4000 \text{ kJ}$$

$$V_{gas} = \frac{4000}{35000} = 0.114 \text{ m}^3$$

$$C = 0.114 \times 36.4 = 4.15 \text{ KZT}$$

$$C = \frac{4.15}{500} = 0.0083 \text{ USD per kWh}$$

The cooling-water cost was estimated based on the official tariff for technical water reported on Kazakhstan's investment portal, equal to 114 KZT/m³ [41]. Since the density of water is approximately 1 tonne/m³, this corresponds to about 114 KZT/tonne, or 0.23 USD/tonne at an exchange rate of 500 KZT/USD. To express the value on a 2026 project basis, the tariff was adjusted using Kazakhstan's 2025 inflation rate for paid services of about 12%, resulting in an updated value of approximately 0.26 USD/tonne [42].

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