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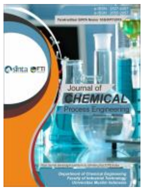

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Process Simulation & Sensitvity Analysis of Cumene Production from an Integrated Alkylation and Transalkylation Reaction

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Key Words: Cumene; Simulation; Sensitivity Analysis; Alkylation; Transalkylation

Abstract

Cumene is a very important petrochemical commodity, mainly to produce phenol and acetone. The overall growth rate for cumene capacity has been healthy, averaging slightly less than 3.5 % per year to reach 18 million metric tons per year in 2017. The purpose of this study is to generate a steady-state process simulation using ASPEN HYSYS version 10 to produce a small capacity of 10 ton/h of cumene with 99.99 wt % product purity. An alkylation reaction of benzene with propylene is carried out for producing cumene by using a zeolites catalyst as modeled by Badger technology. Transalkylation is also integrated into the system for eliminating unwanted products such as p-diisopropyl benzene. The proposed simulation flowsheet provides a good convergence overall result. The preliminary utility consumption obtained from the simulation consists of approximately 0.0418 kton/h of steam, 1.22 kton/h of cooling water, and 450 kW of electrical duty. Optimization is carried out in the simulation by conducting a sensitivity analysis study to find the optimum operating conditions of the alkylation reactor with a dimension of 1.3 m diameter and 4 m of length. The result shows that at an optimum value of B/P molar ratio of 7, reactant temperature of 170 ^{o}C, and reactant pressure of 3 MPa, the selectivity of cumene obtained is at a high value of 0.9446, while the percentage conversion of propylene to cumene obtained is at a high value of 99.99 %.

INTRODUCTION

Cumene is a very important petrochemical commodity, mainly for the production of phenol and acetone [1]. It is usually obtained in the industry by alkylation of benzene with propylene over an acidic catalyst to produce cumene [2]. Transalkylation is also often integrated for cumene production to eliminate unwanted side products such as p-

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diisopropyl benzene, thus increasing the selectivity of cumene [3]. The overall growth rate for cumene capacity between 2000 and 2017 has been healthy, averaging slightly less than 3.5 % per year to reach about 18 million metric tons per year in 2017 [4]. Cumene is a volatile colorless liquid at room temperature with a characteristic sharp, penetrating, and aromatic odor. It is insoluble in water but is soluble in alcohol and many other organic solvents. The physical properties of cumene are shown in Table 1.

Table 1. Physical Properties of Cumene [4]

particular property	description/values
physical state at atmospheric condition	colourless liquid
specific gravity	0.864
boiling point	152 ^{o}C
melting point	-96 ^{o}C
flash point	36 ^{o}C
water solubility	61.3 mgl^{-1}
vapour pressure	4.5 mm Hg at 25 ^{o}C

The demand for cumene is largely dependent on the performance of phenol's derivatives, which have resulted in healthy growth rates [1]. Cumene is also used in the manufacture of acetophenone, methyl styrene, and other chemicals commonly found in home cleaning products [5]. Minor uses of cumene include as a constituent of some petroleum-based solvents, as raw material for peroxides, and as oxidation catalysts such as polymerization catalysts for acrylic and polyester-type resins [6].

OBJECTIVE

The objective of this research is to generate a steady-state process simulation using simulation software ASPEN HYSYS version 10 for the production of small-capacity cumene from an integrated catalyzed alkylation and transalkylation reaction using peng-Robinson as a fluid package. The simulation flowsheet is developed based on reference from an official cumene production licensor, Badger's Technology [4]. In the alkylation stage, benzene reacts with propylene to produce cumene, while a side reaction also occurs simultaneously where propylene reacts with cumene to produce p-diisopropyl benzene as the unwanted product, thus, sensitivity analysis study to investigate the optimum operating conditions of the alkylation reactor in producing the highest amount of cumene while minimizing the unwanted product.

The production of cumene in this present study is designed at a small capacity of 10 ton/h. The product specification of cumene consists of a minimum 99.99 wt% of cumene purity. The raw materials used for the alkylation process are benzene with high percentage purity (96 mol% benzene) and propylene which consist of 5 mol% propane impurity (95 mol% propylene and 5 mol% propane). The estimated benzene feed requirement is 600 kmol/h and the propylene feed requirement is 100 kmol/h, where the benzene to propylene feed molar ratio is initially chosen at 6. Table 2 shows the summarised specification of raw materials and products.

Table 2. Feed & Product Specification [4]

components particular	values
cumene	> 99.99 wt%
benzene	> 96 mol%
propylene	> 95 mol% (5 mol% n-C_3 impurity)

METODOLOGY

The methodology in conducting this research began with developing the required research specification, which serves as the primary guideline for the pathway of this study. All technical design basis such as simulation flowsheet, process description, manufacturing route, reactor design, separation & purification system, and utility specification is then developed concerning credible literature sources. A simulation flowsheet using simulation software ASPEN HYSYS version 10 is then developed based on the technical design basis until convergence status has been reached. If the convergence status of the simulation flowsheet has not been reached, then both simulation configuration and design basis input need to be re-checked until convergence status is obtained. Optimization is also carried out by conducting a sensitivity analysis study to investigate the best-operating conditions for the alkylation reactor. Figure 1 shows the research algorithm flowchart.

MANUFACTURING ROUTE

Commercial production of cumene is by Friedel–Craft's alkylation of benzene with propylene [7]. The original route for manufacturing cumene was by alkylation of benzene in the liquid phase using sulfuric acid as a catalyst, but because of the complicated neutralization and recycling steps required, together with corrosion problems, this process has been largely replaced [7]. As an alternative, solid phosphoric acid supported on alumina was used as the catalyst for the cumene production method [2].

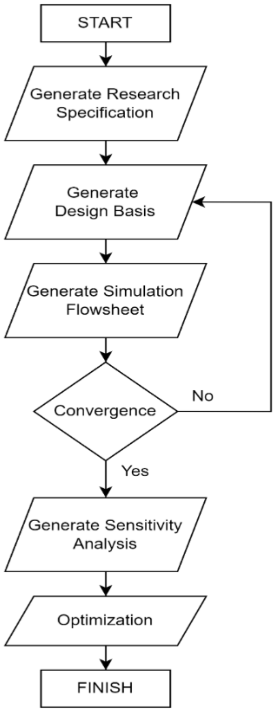

Figure 1. Research Algorithm Flowchart

In 1976, an improved cumene process that uses aluminum chloride as a catalyst was developed [2]. The overall conversion of cumene for this process can be as high as above 90 % [4]. However, such materials usually introduced various problems such as corrosion, safety hazards, and sustainability risks [2]. In recent years, industrial alkylation processes for cumene production reveals that environmentally friendly and efficient zeolites are more frequently being used as catalysts for this reaction [8]. The production of cumene by the Friedel–Crafts alkylation of benzene with propylene, is an irreversible and exothermic reaction (equation. 1) [9].

Propylene + Benzene → Cumene…………………(1)
Propylene + Cumene → p-diisopropyl benzene…. (2)
p-diisopropyl benzene + Benzene ⇌ Cumene…….(3)

However, during the alkylation process, side reactions may also occur resulting in the undesirable formation of p-diisopropyl benzene (equation 2) [10]. Nevertheless, the formation of p-diisopropyl benzene can be partially overturned by integrating a transalkylation reaction into the system, where p-diisopropyl benzene is converted back to cumene in a reversible reaction (equation 3) [10]. In this present study, simulation flowsheet configuration is developed based on Badger Cumene Technology licensor and by using a common zeolites catalyst [4].

PROCESS DESCRIPTION

In the alkylation process for the production of the industrial scale of cumene, benzene and propylene serve as the basic raw material. Benzene is chosen as the excess reactant while propylene is chosen as the limiting reactant. Benzene and propylene are pumped by using an individual transfer pump from a dedicated storage tank and mixed within the piping system routed to the feed-effluent heat exchanger. This is to ensure all reactants, which are benzene and propylene, are completely heated up to the desired temperature as per specification before entering the alkylation reactor. All reactants exiting the feed-effluent heat exchanger are then transferred to the alkylation reactor, in which a reaction between benzene and propylene to produce cumene takes place. Other than the main reaction, side reaction also occurs in the alkylation reactor, in which propylene and cumene react to form p-diisopropyl benzene as the unwanted side product. The product or reactor effluent obtained from the alkylation reactor, which is in liquid phase condition, is cooled via the feed-effluent heat exchanger. Figure 2 & 3 shows the simplified process flow diagram and simulation flowsheet for the manufacturing of cumene.

Assuming full conversion of propylene as it was chosen as the limiting reactant, thus the reactor effluent consists of propane, benzene, p-diisopropyl benzene, and cumene. In this case, 3 distillation column is used for the separation & purification process.

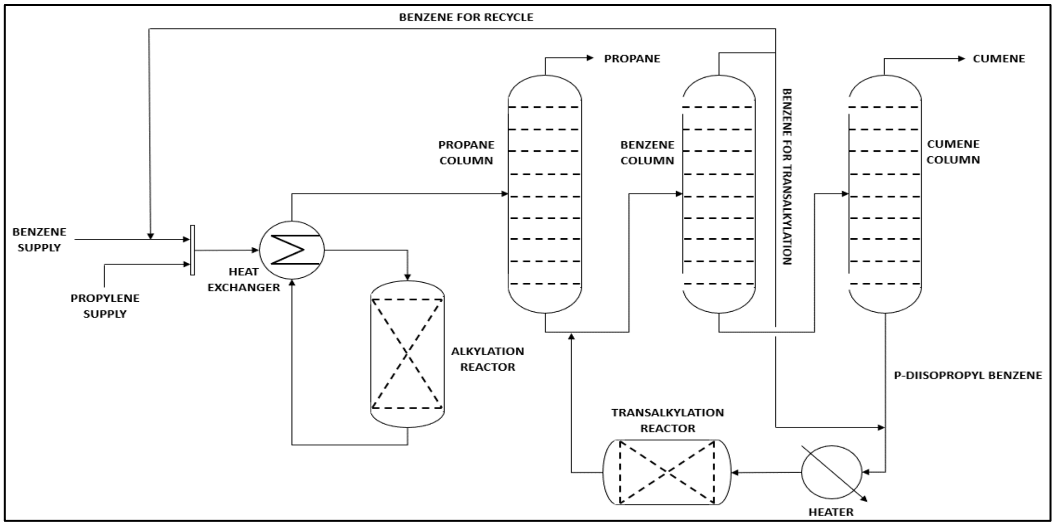

Figure 2. Simplified Process Flow Diagram for Cumene Manufacturing

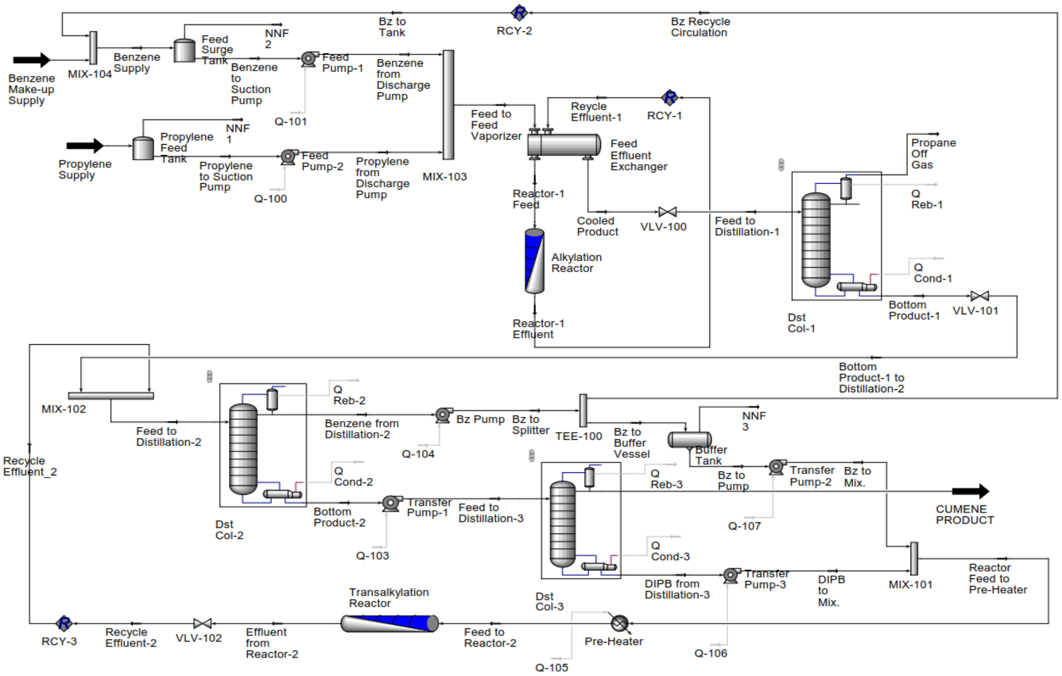

Figure 3. Simulation Flowsheet for Cumene Manufacturing

The first distillation column separates the lightest component, which is propane, from the rest of the mixture. Propane exiting as off gas from the top column and can be re-used as fuel gas for utility systems in the plant, such as for boiler's fuel consumption. The second distillation column separates benzene from the remaining mixtures of p-diisopropyl benzene and cumene. Benzene exits from the top column as liquid and is recycled by a benzene booster pump for re-used as feed inside the storage tank and as feed for the transalkylation process. The remaining mixture which consists of cumene and p-diisopropyl benzene obtained from the bottom part of the second distillation column is then pumped to the final distillation column to separate between cumene and p-diisopropyl benzene. Cumene exits from the top column as liquid and is stored in the product storage tank for delivery, while p-diisopropyl benzene exits from the bottom column. In this present study, all distillation column uses steam as a heating medium in the bottom column reboiler and cooling water as a cooling medium in the top column condenser.

In the transalkylation section, p-diisopropyl benzene exiting from the final distillation column and a portion of the recycled benzene obtained from the second distillation column are both pumped by using an individual transfer pump and mixed together at a dedicated manifold. This mixture is then routed through a pre-heater and then directed to a transalkylation reactor, where p-diisopropyl benzene is partially converted into cumene in a reversible reaction with benzene. The product from the transalkylation reactor is recycled and mixed with the bottom product of the first distillation column before being routed to the second distillation column for benzene purification and separation.

REACTION KINETICS

According to the manufacturing route, the main reaction used in the industrial-scale production of cumene is the alkylation of benzene with propylene in the presence of a catalyst [10]. However, there is a side reaction occurring during this alkylation process, in which propylene reacts with cumene to produce p-diisopropyl benzene as the unwanted side product [8]. The formation of p-diisopropyl benzene can be partially overturned by using a transalkylation process, in which p-diisopropyl benzene is converted back to cumene by reacting with benzene in the presence of a catalyst [3]. However, the nature of this reaction is reversible, where cumene can also be converted back to p-diisopropyl benzene and benzene depending on the operating temperature and pressure of the reaction [3]. The overall reaction occurring in the production of cumene is represented by reactions 1 to 4 as shown in the description below (reaction 3 as shown in equation 6 is the forward reaction of transalkylation, while reaction 4 as shown in equation 7 is the reverse reaction of transalkylation) [10].

Reaction 1: $C_3H_6 + C_6H_6 \rightarrow C_9H_{12}$ ……………….(4)
Reaction 2: $C_3H_6 + C_9H_{12} \rightarrow C_{12}H_{18}$……………...(5)
Reaction 3: $C_{12}H_{18} + C_6H_6 \rightarrow 2\ C_9H_{12}$……………(6)
Reaction 4: $2\ C_9H_{12} \rightarrow C_{12}H_{18} + C_6H_6$…………………..(7)

The kinetic parameters and rate constants of the reactions considered in this present study are summarised and shown in Table 3.

Table 3. Rate Constant Parameters [10]

Reaction	Rate Constants
Alkylation [Reaction 1]	$K_1 = 6510\ e^{(-52564/RT)}$
Unwanted Reaction [Reaction 2]	$K_2 = 450\ e^{(-55000/RT)}$
Transalkylation (Forward Reaction) [Reaction 3]	$K_3 = 2.529 \times 10^8\ e^{(-100000/RT)}$
Transalkylation (Reverse Reaction) [Reaction 4]	$K_4 = 3.877 \times 10^9\ e^{(-127240/RT)}$

REACTOR DESIGN

The reaction for the production of cumene is commonly carried out in an adiabatic fixed bed reactor consisting of catalyst pellets, commonly zeolite catalyst [11]. In this present study, two dedicated catalytic reactors are used, each for the alkylation and transalkylation process. In the alkylation reactor, the common best practice for the operating temperature and pressure is within the range between 150 ^oC to 230 ^oC and 2.5 MPa to 3.5 MPa, while the molar ratio of benzene to propylene feed is within the range between 5 to 8 [8]. An excess amount of benzene is usually required in the reactor for the following reasons, for absorbing heat generated by exothermic reactions in the rector, for enhancing the selectivity of the cumene reaction over the unwanted side reaction, and for suppressing the reaction between propylene molecules, which produces higher linear hydrocarbons [12]. In the transalkylation reactor, the common best practice for the operating temperature and pressure is within the range between 140 ^oC to 150 ^oC and 2.5 MPa to 3.5 MPa, while the molar ratio for benzene to p-diisopropyl feed is within the range between 20 to 30 [8]. All reactants in the alkylation and transalkylation reactor are in the liquid phase [8].

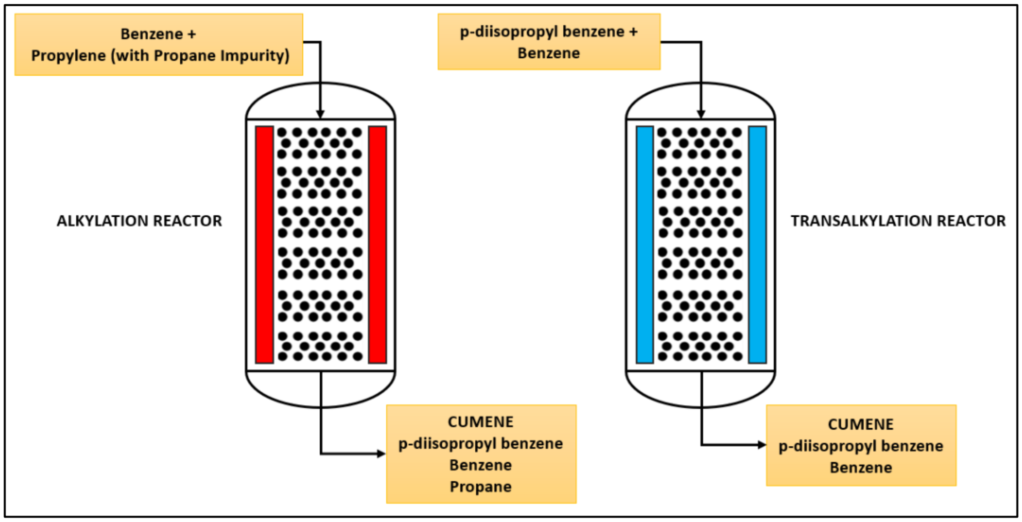

Figure 4. General Schematic of Fixed-bed Catalytic Reactor

In this present study, for the simplification purpose of the alkylation process, a single adiabatic catalytic fixed-bed reactor is used (as shown in Figure 4) with a diameter of 1.3 m and a total length of 4 m. The inlet temperature feed to the alkylation reactor is initially chosen at 170 ^{o}C and operating pressure of 3.2 MPa. The molar ratio of benzene to propylene is initially chosen at 6. Asides from that, for the transalkylation process, a single adiabatic catalytic fixed-bed reactor is used (as shown in Figure 4) with a diameter of 1.3 m and a total length of 4 m. The inlet temperature feed to the transalkylation reactor is chosen at 145 ^{o}C and operating pressure of 3.1 MPa. The molar ratio of p-diisopropyl benzene to benzene is chosen at 25. The alkylation and transalkylation process is enhanced by zeolites catalyst with the general specification as summarised in Table 4.

Table 4. Zeolites Catalyst Specification [8]

catalyst particular	values
particle density, kg/m^3	1000
particle size, mm	3
void fraction	0.4

The flowrate of reactant feed entering the alkylation reactor is approximately 700 kmol/h, consisting of 100 kmol/h propylene feed and 600 kmol/h benzene feed. The reactant enters the alkylation reactor at an operating temperature of 170 ^{o}C and exits the alkylation reactor at an operating temperature of 242.5 ^{o}C. The reaction of alkylation of benzene and propylene is exothermic and heat is released to the surroundings, thus causing an increase in the temperature. Figure 6 shows the relation between the temperature of the fluid mixture along the alkylation reactor. The inlet pressure to the alkylation reactor is set at 3.2 MPa, while the pressure drop across the alkylation reactor obtained is approximately 2 kPa. The operating pressure decreases linearly due to the pressure drop effect along the alkylation reactor as shown in Figure 7. The percentage conversion of propylene to cumene as obtained from the simulation is approximately 99.99 %. In this case, propylene serves as the limiting reactant while benzene is the excess reactant. The selectivity of cumene is obtained at 0.9442. Figure 5 shows the molar flowrate of all reactants and products across the alkylation reactor, while Table 5 shows the summarised results of molar composition entering and exiting the alkylation reactor.

Table 5. Alkylation Reactor Molar Fraction

Components	Molar Fraction / Reactor Feed	Molar Fraction / Reactor Effluent
Benzene	0.8249	0.7982
Propylene	0.1357	0.0000
Propane	0.0072	0.0084
Cumene	0.0321	0.1926
p-diisopropyl benzene	0.0000	0.0008

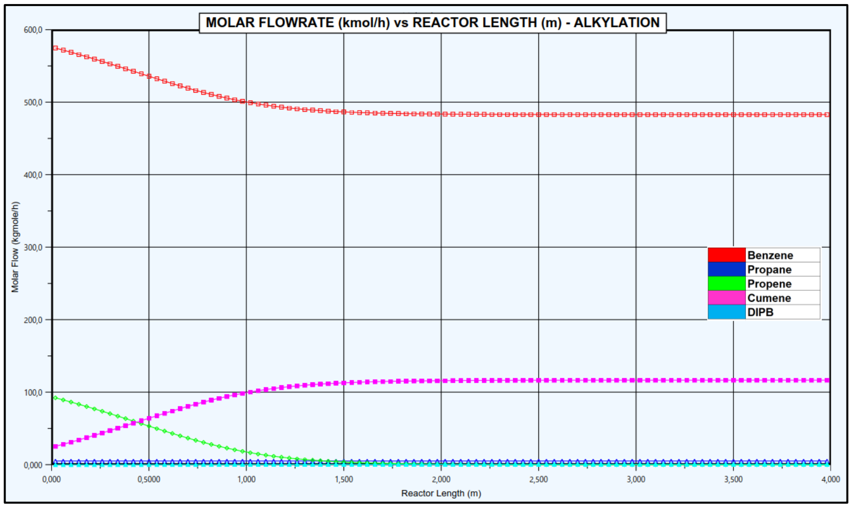

Figure 5. Graph of Molar Flowrate vs. Reactor Length for Alkylation

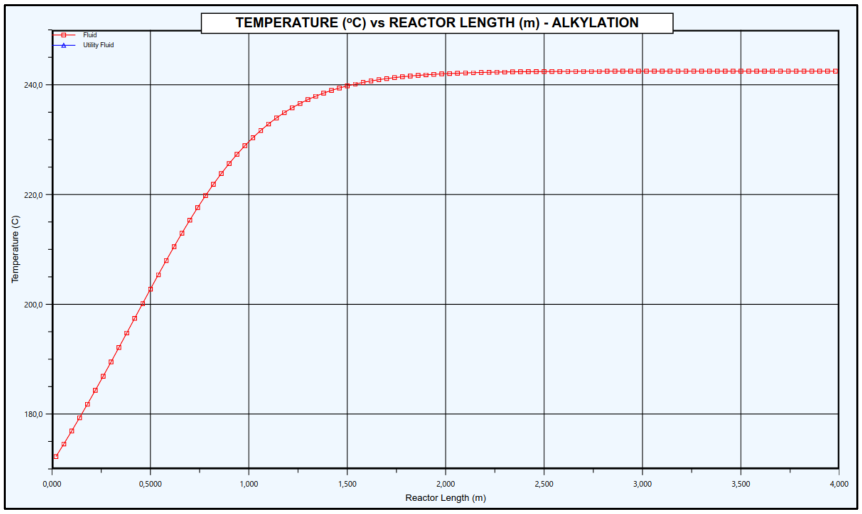

Figure 6. Graph of Temperature vs. Reactor Length for Alkylation

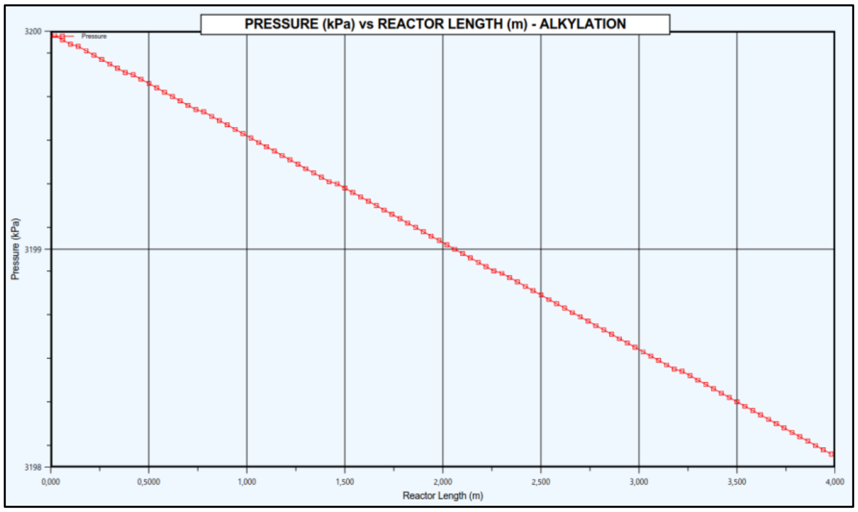

Figure 7. Graph of Pressure vs. Reactor Length for Alkylation

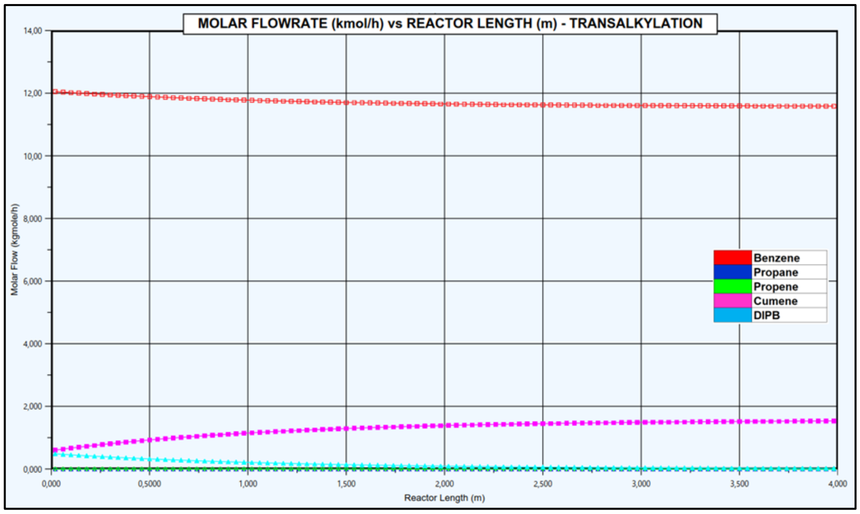

Figure 8. Graph of Molar Flowrate vs. Reactor Length for Transalkylation

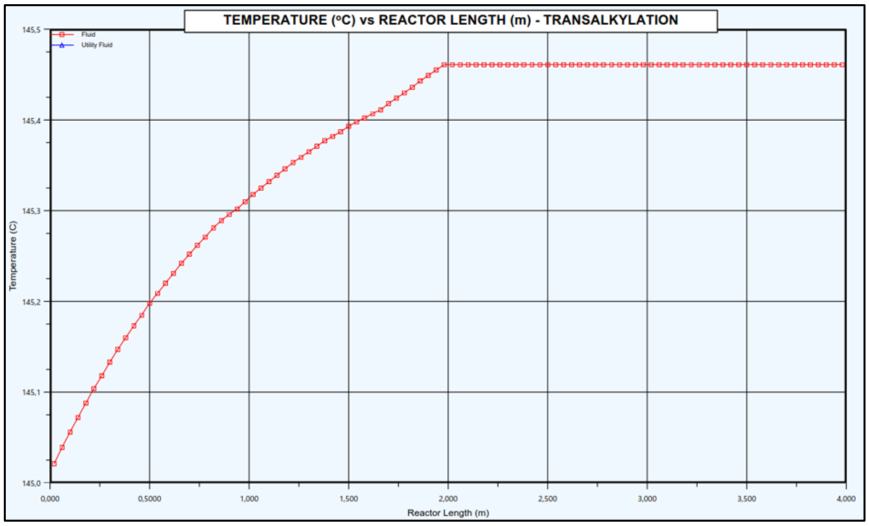

Figure 9. Graph of Temperature vs. Reactor Length for Transalkylation

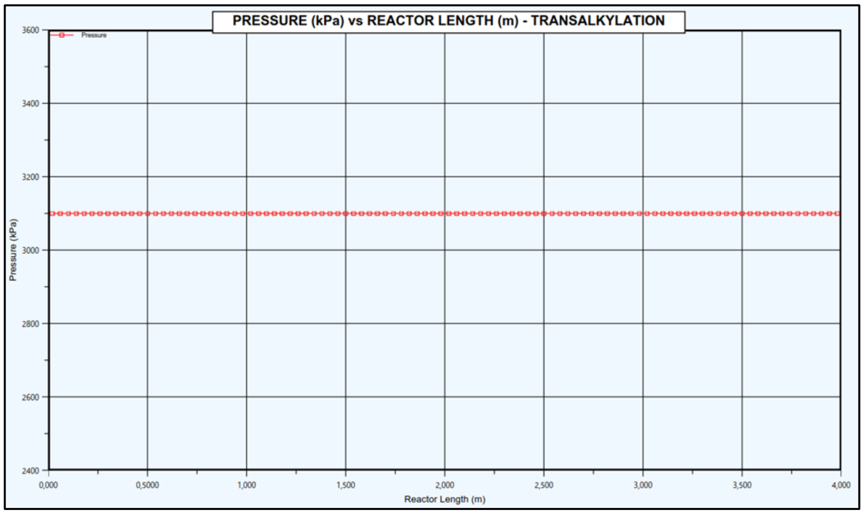

Figure 10. Graph of Pressure vs. Reactor Length for Transalkylation

The flowrate of reactant feed entering the transalkylation reactor is approximately 13.14 kmol/h, consisting of around 91.86 mol% benzene, 3.81 mol% p-diisopropyl benzene, 0.01 mol% propane, and 4.32 mol% cumene. The reactant enters the transalkylation reactor at an operating temperature of 145 ^{o}C and exits at an operating temperature of 145.5 ^{o}C as shown in Figure 9. The increase in temperature is not significant, only at 0.5 ^{o}C increment rise. The inlet pressure of the feed reactant is approximately 3.1 MPa, while the pressure drop across the transalkylation reactor is very small, around 0.005 kPa. Therefore, the inlet and outlet pressure across the transalkylation reactor is assumed to be the constant for this particular capacity of feed inlet. Figure 10 shows the relation between pressure and reactor length for the transalkylation reactor. The percentage conversion of p-diisopropyl benzene to cumene as obtained from the simulation is approximately 96.40 %. In this case, p-diisopropyl benzene serves as the limiting reactant while benzene is the excess reactant. The selectivity of cumene is obtained at 0.9980. Figure 8 shows the molar flowrate of all reactants and products across the transalkylation reactor, while Table 6 shows the summarised results of molar composition entering and exiting the transalkylation reactor.

Table 6. Transalkylation Reactor Molar Fraction

Components	Molar Fraction / Reactor Feed	Molar Fraction / Reactor Effluent
Benzene	0.9186	0.8819
Propylene	0.0000	0.0000
Propane	0.0001	0.0001
Cumene	0.0432	0.1167
p-diisopropyl benzene	0.0381	0.0014

UTILITY SPECIFICATION

The scope of utility demand in this present study is limited to only steam, cooling water, and electrical duty demand. All values presented in this study are only preliminary and serve as the minimum baseline for the cumene production design of 10 ton/h capacity feasibility study. The detail of the utility demand is explained as the following:

1. The steam specification used is steam at saturated pressure of 30 bar (saturated temperature of 234 ^{o}C) with a latent heat value of 1795 kJ/kg. Steam supply is needed for heating purposes, especially for all distillation column's reboiler and transalkylation reactor's pre-heater. The preliminary steam demand as shown by the simulation result is approximately 0.0418 kton/h.
2. The cooling water specification used is at a temperature supply of 32 ^{o}C and a maximum temperature return of 45 ^{o}C. The specific heat capacity of water used for the estimation of cooling water demand is taken as 4.313 kJ/kg.K. Cooling water supply is needed for all cooling purposes, especially for all distillation column condensers. The preliminary cooling water demand as obtained from the simulation result is approximately 1.22 kton/h.
3. Electrical duty demand is limited to rotating equipment such as pumps, while other auxiliary components have not been included. Hence, the value represented in this present study serves as preliminary value only. The preliminary electrical duty demand for all pumps is approximately 450 kW.

Table 7 shows the summarised preliminary utility requirement for the production of cumene at 10 ton/h capacity.

Table 7. Preliminary Utility Requirement

Utility Particular	Values
Steam (kton/h)	0.0418
Cooling Water (kton/h)	1.22
Electrical Duty (kW)	450

SEPARATION & PURIFICATION

The alkylation reactor effluent consists of a mixture of impurities with cumene as the main product. Assuming full conversion of propylene as it was chosen as the limiting reactant, thus the reactor effluent consists of propane, benzene, p-diisopropyl benzene, and cumene. Hence, cumene is separated from the mixture of impurities by the method of distillation, based on the difference in boiling point [13]. There are 3 distillation columns considered in this design (from Figure 11), with the lightest component shall be separated in the first place [13].

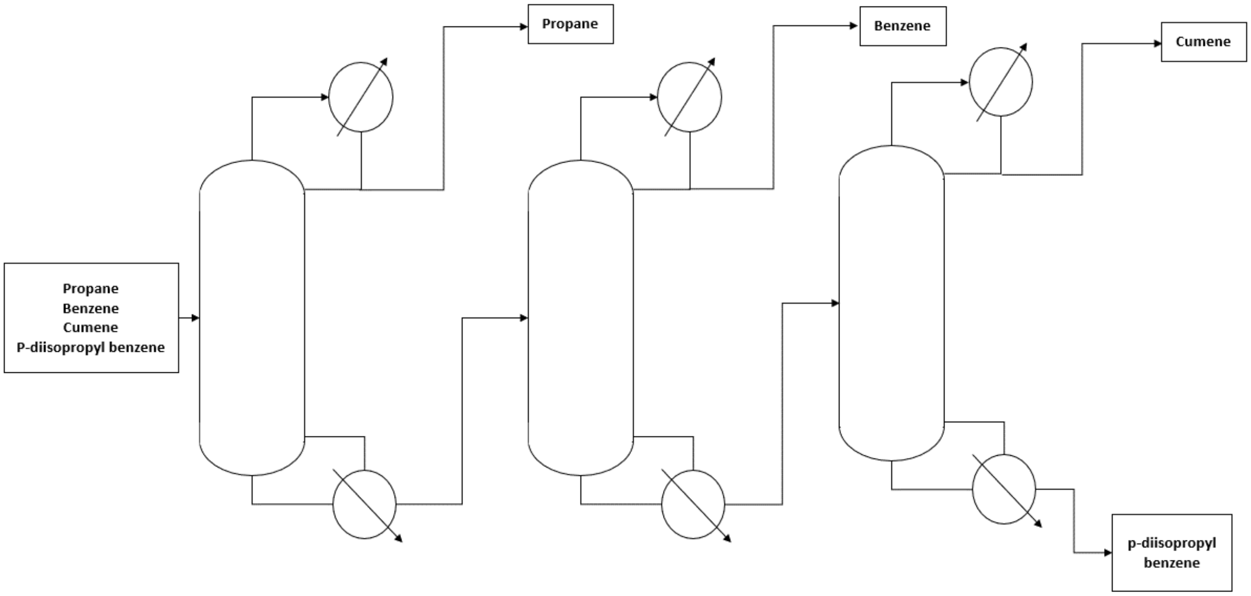

Figure 11. Distillation System in Cumene Manufacturing

The first distillation column has the objective to separate propane from the feed mixture as off-gas exiting from the top column. The top column is set at a pressure of 1500 kPa and a temperature of 43.86 °C, while the bottom column is set at a pressure of 1600 kPa and a temperature of 219.20 °C. The off-gas composition obtained consists of 99 wt% propane. The first distillation column consists of 10 trays and feed enters at the 8th stage. The second distillation column has the objective to separate benzene from the feed mixture as the top column liquid product. The top column is set at a pressure of 100 kPa and temperature of 80.95 °C, while the bottom column is set at a pressure of 120 kPa and temperature of 160.50 °C. Benzene composition obtained is at 96 mol% purity and mostly to be recycled to feed storage tank via a recycling pump for re-use purposes, while only a small portion is utilized for transalkylation purposes. The second distillation column consists of 10 trays and feed enters at the 5th stage. The third distillation column has the objective of cumene product purification, which is to separate cumene from p-diisopropyl benzene. Cumene is obtained at the top column product as liquid with a purity of 99.99 wt% cumene, while p-diisopropyl benzene is obtained as the bottom product and is routed to the transalkylation reactor for transalkylation reaction with benzene. The top column is set at pressure 100 kPa and temperature 153.10 °C, while the bottom column is set at pressure 110 kPa and temperature 212.40 °C. The third distillation column consists of 10 trays and feed enters at the 5th stage.

SENSITIVITY ANALYSIS

In the alkylation process, benzene reacts with propylene to produce cumene, while a side reaction also occurs simultaneously where propylene reacts with cumene to produce p-diisopropyl benzene as the unwanted product. To maximize the production of cumene while minimizing the production of p-diisopropyl benzene, sensitivity analysis has been carried out to investigate the best-operating conditions for the alkylation reactor. The dimension of the alkylation reactor with a diameter of 1.3 m and length of 4 m, catalyst zeolite specification (reference Table 4), and propylene feed molar flowrate at 100 kmol/h are selected as constant parameters. The optimum percentage conversion of propylene to cumene and selectivity of cumene can be obtained by optimizing the 3 parameters within the alkylation reactor as shown by the following:

1. Benzene to propylene (B/P) feed molar ratio
2. Temperature of reactant to alkylation reactor
3. Pressure of reactant to alkylation reactor

In this present study, the B/P molar ratio is varied from 4 to 12, the temperature of reactant to alkylation reactor is varied from 120 °C to 200 °C, and the pressure of reactant to alkylation reactor is varied from 2.5 MPa to 3.5 MPa. The combination of values from the 3 corresponding parameters that yield the optimum percentage conversion of propylene to cumene and selectivity of cumene is selected as the best-operating conditions for the alkylation reactor. However, the results obtained from this sensitivity analysis are limited to the particular size of the alkylation reactor and the zeolites catalyst specification that are chosen within this study.

Effect of Alkylation Reactant B/P molar ratio on (%) Conversion & Selectivity

In this sensitivity analysis, the B/P molar ratio of the reactant to the inlet of the alkylation reactor is varied from 4 to 12. Other parameters such as reactant temperature at 170 ^{o}C and reactant pressure at 3.2 MPa entering the alkylation reactor are kept constant. The results obtained (from Figure 12) show that from the B/P molar ratio of 4 to 7, the selectivity of cumene increases from 0.9421 to an optimum value of 0.9446. Initially, the selectivity increased due to the increase in the amount of cumene produced as the reaction started to occur. At this range of B/P molar ratio, the amount of production of cumene is greater than the amount of production of p-diisopropyl benzene (unwanted product). However, the graph then descends from the optimum value (at a B/P molar ratio of 7) until it reaches a selectivity value of 0.9109 at a B/P molar ratio of 12. As the B/P molar ratio increased beyond 7, the amount of production of cumene is lesser than the amount of production of p-diisopropyl benzene (unwanted product), resulting in a gradual decrease in the selectivity of cumene. Another contributing factor to the declining selectivity of cumene is that the increase in the formation of p-diisopropyl benzene blocked both benzene and propylene from reaching the catalytic pores of the catalyst [11]. Thus, reducing the feasibility of the alkylation reaction of benzene and propylene in producing cumene.

On the other hand, from a B/P molar ratio of 4 to 7 (from Figure 14), the percentage conversion of propylene to cumene remains constant at a very high value of 99.99%, while from a B/P molar ratio of 7 to 12, the percentage conversion of propylene to cumene decreased gradually until it reaches 96.33%. This result is consistent with the analysis of the selectivity of cumene against the change in the B/P molar ratio (from Figure 12). As the B/P molar ratio increased from 4 to 7, the majority of the propylene reacted with benzene to form cumene in an alkylation reaction, resulting in a high percentage conversion of propylene to cumene. However, from a B/P molar ratio of 7 to 12, most of the propylene instead reacts in a side reaction with cumene to form p-diisopropyl benzene (unwanted product), thus resulting in the gradual decrease of the percentage conversion of propylene to cumene. Therefore, from the results of the selectivity of cumene and the percentage conversion of propylene to cumene, the optimum B/P molar ratio is chosen to be at 7.

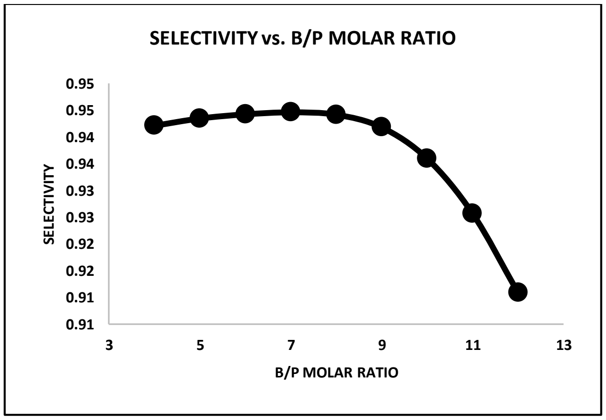

Figure 12. Graph of Selectivity vs. B/P Molar Ratio

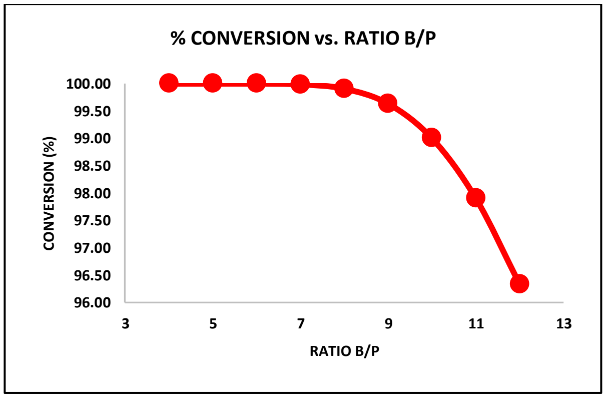

Figure 13. Graph of Conversion vs. B/P Molar Ratio

Effect of Alkylation Reactant Temperature on (%) Conversion & Selectivity

In this sensitivity analysis, the reactant temperature to the inlet of the alkylation reactor is varied from 110 ^{o}C to 200 ^{o}C. Other parameters such as the B/P molar ratio at 7 and reactant pressure at 3.2 MPa entering the alkylation reactor are kept constant. The results obtained (from Figure 14) show that as the temperature increased from 110 ^{o}C to 170 ^{o}C, the selectivity increased from 0.6969 to an optimum value of 0.9446. However, from a temperature of 170

^{o}C to 200 ^{o}C, the selectivity gradually decreased until it reaches a value of 0.9242. Initially, the selectivity increased due to the increase in the amount of cumene produced as the reaction started to occur. At this range of temperature, the production of cumene is greater than the production of the unwanted product, p-diisopropyl benzene. However, beyond the temperature of 170 ^{o}C, the selectivity of cumene began to slightly decrease as the production of cumene is lesser than the production of the unwanted product, p-diisopropyl benzene. The alkylation of benzene with propylene in producing cumene is an exothermic reaction, where a low-temperature reaction favors the production of cumene [11]. Conversely, an increase in temperature favors the formation of p-diisopropyl benzene [3]. Another contributing factor to the declining selectivity of cumene is that the increase in the formation of p-diisopropyl benzene blocked both benzene and propylene from reaching the catalytic pores [11]. Thus, reducing the feasibility of the alkylation reaction of benzene and propylene in producing cumene.

On the other hand, from a temperature of 110 ^{o}C to 170 ^{o}C (from Figure 15), the percentage conversion of propylene to cumene increased from 73.73 % to an optimum value of 99.99 %. However, from a temperature of 170 ^{o}C to 200 ^{o}C, the percentage conversion of propylene to cumene slightly decreased from 99.99 % to 97.80 %. This result is consistent with the analysis of the selectivity of cumene against the change in the operating temperature (from Figure 14). As the temperature increases from 110 ^{o}C to 170 ^{o}C, the majority of the propylene reacted with benzene to form cumene in an alkylation reaction, resulting in a high percentage conversion of propylene to cumene [2]. However, from the temperature of 170 ^{o}C to 200 ^{o}C, most of the propylene instead reacts in a side reaction with cumene to form p-diisopropyl benzene (unwanted product), resulting in a gradual decrease of the percentage conversion of propylene to cumene. Therefore, from the results of the selectivity of cumene and the percentage conversion of propylene to cumene, the optimum temperature is chosen to be at 170 ^{o}C.

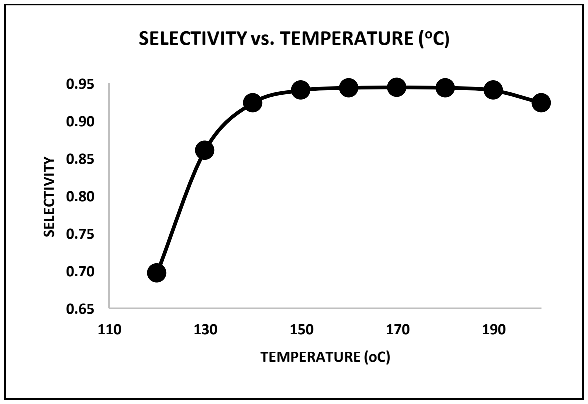

Figure 14. Graph of Selectivity vs. Temperature

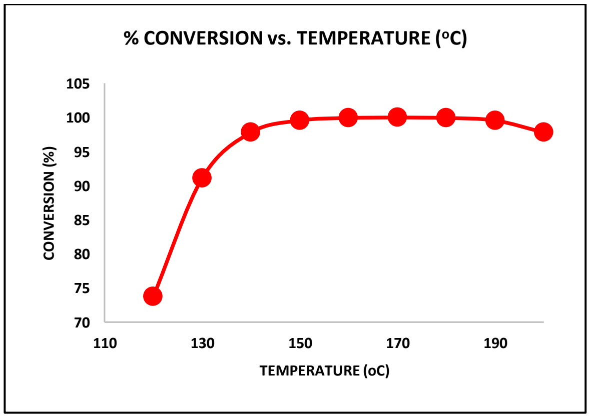

Figure 15. Graph of Conversion vs. Temperature

Effect of Alkylation Reactant Pressure on (%) Conversion & Selectivity

In this sensitivity analysis, reactant pressure to the inlet of the alkylation reactor is varied from 2500 kPa to 3500 kPa. Other parameters such as the B/P molar ratio at 7 and reactant temperature at 170 ^{o}C entering the alkylation reactor are kept constant. The results obtained (from Figure 16 & 17) shows that as the pressure is increased from 2500 kPa to 3500 kPa, the selectivity of cumene remains constant at approximately 0.9446, while the percentage conversion of propylene to cumene remain constant at 99.99 %. At this range of pressure, the amount of cumene production (main product) and p-diisopropyl benzene production (unwanted side product) is constant, thus resulting in a constant selectivity of cumene and a constant percentage of conversion of propylene to cumene. At higher operating pressure, one of the drawbacks is that the capital expenditure would be higher as equipment material needs to be thicker and stronger while operating expenditure would be higher as the feed pump needs to be operating at a higher discharge value. However, choosing a very low-pressure operation is also not recommended as reactant fluid has to be highly pressurized to ensure that it is in the liquid phase for both alkylation and transalkylation reaction [8]. Therefore, an optimum operating pressure according to the best common practice is chosen to be at 3000 kPa [12].

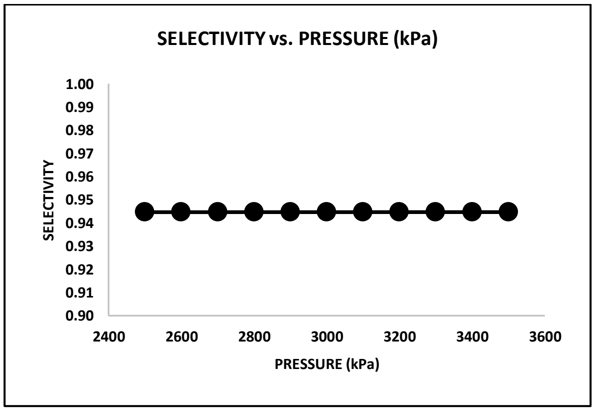

Figure 16. Graph of Selectivity vs. Pressure

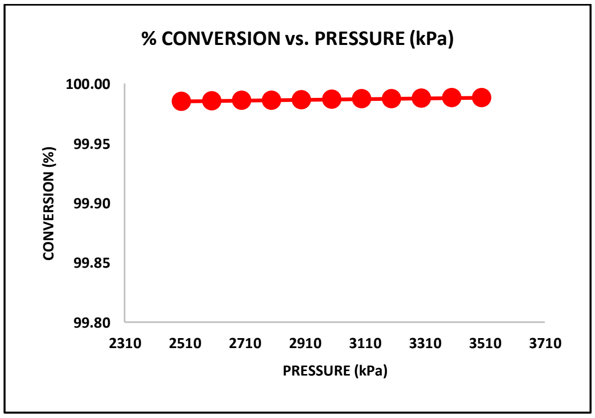

Figure 17. Graph of Conversion vs. Pressure

CONCLUSION

The following conclusion for this present study are summarised within the points as shown below:

1. The proposed scheme for the production of cumene from the alkylation of benzene and propylene, integrated with the transalkylation of p-diisopropyl benzene and benzene for the elimination of side product, provided an overall convergent simulation result for a small production capacity of 10-ton/h with purity product of 99.99 wt%. The estimated preliminary utility requirement for the corresponding capacity of production consists of 0.0418 kton/h of steam, 1.22 kton/h of cooling water, and 450 kW of electrical duty.
2. Sensitivity analysis conducted for investigating the optimum operating conditions of the alkylation reactor shows that the B/P molar ratio and temperature of reactant feed have a major effect on the selectivity of cumene and the percentage conversion of propylene to cumene. The optimum value obtained for the B/P molar ratio is at 7 and for the temperature of reactant feed is at 170 ^{o}C. However, variation in the reactant feed pressure shows no significant impact on the selectivity of cumene and the percentage conversion of propylene to cumene. Nevertheless, high operating pressure at 3 MPa is recommended as per common best practices for ensuring only liquid-phase reactions occur in both the alkylation and transalkylation reactor. At this corresponding optimum value of B/P molar ratio, reactant temperature, and reactant pressure, the selectivity of cumene is obtained at 0.9446 while the percentage conversion of propylene to cumene is obtained at 99.99 %.

ABBREVIATION

B/P	benzene to propylene feed molar ratio
X_B	molar fraction of benzene
X_C	molar fraction of cumene
X_D	molar fraction of p-diisopropyl benzene
E	activation energy, kJ/kmol
HP	high pressure
K_1	first-order reaction constant in reaction 1, s^{-1}
K_2	first-order reaction constant in reaction 2, s^{-1}
K_3	forward reaction constant in reaction 3, $kmol/m^3.s$
K_4	reverse reaction constant in reaction 4, $kmol/m^3.s$
R	gas constant, 8.316 kJ/kmol.K
T	temperature, K

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