

CHEE-4844

Design of an Alkylation Packed Bed Reactor for Cumene Production with Aspen HYSYS V10

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EXECUTIVE SUMMARY

Cumene can be manufactured from the gas-phase alkylation reaction between propylene and benzene in a packed bed reactor in the presence of a zeolite catalyst. The feed ratio of benzene to propylene in cumene synthesis varies between 2:1 to 7:1 and diisopropylbenzene (DISB) is a byproduct of the alkylation reaction.

The objective of this report is the design of two gas-phase alkylation reactor variants that achieve a 95% cumene yield from propylene within design constraints. The constraints include a minimum B/P feed ratio of 5:1, a maximum reactor volume of 20 m³, and a maximum pressure drop of 100 kPa across each reactor. The propylene feed contains a 5 mol.% propane impurity, and the total propylene supplied is 104 kg-mol./h. In addition, each reactor variant is constrained to the utilization of a beta-zeolite derivative catalyst (QZ-2500H) with a density of 2000 kg/m³ and a particle diameter of 1 mm

A variant of the packed bed reactor was designed as a low-temperature operation adiabatic PFR unit and the other as high-temperature operation inter-stage cooled adiabatic PFR reactors. Both reactors were designed to each achieve a 95% cumene yield for the same feedstock shown. The lower temperature adiabatic reactor had an operational volume of 20 m³, while the higher temperature unit has total volume of 10.5 m³.

The low temperature variant had an operating cost \$303,800 lower than the high temperature variant due to the additional cooling requirements of the higher temperature variant. Both reactor variants produce approximately 11250.5 kg/h of cumene. The annualized credit from cumene at a selling price of \$1.47/kg [15] is \$137,351,594 for both reactors. The total annualized operating costs of the low temperature variant is \$45,589,925 greater than the credit from cumene sold; the operating costs are \$46,172,833 greater for the high temperature variant.

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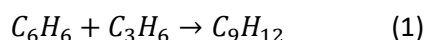
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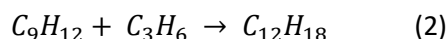
1. BACKGROUND INFORMATION

Cumene, otherwise known as isopropyl benzene, is a high-octane blending component in aviation fuel [1], a thinner for paints, and solvent for fat and resins [2]. The compound is primarily used as an intermediate in the production of phenol and acetone; 95% [2] to 99% [1] of the 12.4 million metric tons produced in 2011 [3] was the raw material for the manufacture of phenol. Cumene is the main product of a modified Friedel-Crafts alkylation reaction between propylene and benzene in an acid catalyst, such as solid phosphoric acid (SPA) or hydrogen fluoride [1] and aluminum chloride [4]. The equation representing the alkylation reaction is given by Equation 1. Alternatively, the compound can be manufactured from the distillation of coal tar and petroleum fractions; crude oil contains 0.1 wt.% to 1 wt.% cumene [2].



The manufacturing process involves pressurization, heating, and mixing of propylene and benzene streams to specifications governed by the selected catalyst. The exothermic reaction occurs in a packed bed gas phase reactor [3]; the reactor is typically divided into four packed catalyst beds contained in a single reactor shell [1]. In addition to the principal alkylation reaction, acidic catalysts promote olefin oligomerization, poly alkylation, and hydride transfer side reactions [1]; these result in the production of heavy alkylates, di-isopropyl benzene (DISB), and di-phenyl propane respectively. Therefore, the reactor effluent contains unreacted benzene, cumene, and a mixture of the aforementioned by-products. The most cited by-products of the alkylation of benzene with propylene are DISB [3] and tri-isopropyl benzene (TISB); typical alkylation reactor effluents contain 5-10 wt.% DISB and TISB [1]. Equation 2 shows the poly-alkylation reaction between cumene and propylene, leading to the formation of DISB. Unreacted benzene is recovered from the effluent stream by distillation and recycled to the alkylation reactor [4]; the main by-products are separated from cumene with an additional distillation column [3]. The quality of the cumene product from any specific manufacturing process is strongly influenced by the specific contaminants present in the feedstock. A cumene purity of 99.97wt.% can be obtained from a minimal of 99.5wt.% polymer-grade propylene and 99.8wt% benzene [1]. However, propane impurities in the propylene feed stream are common; typical propylene feed into the alkylation reactor contains 5mol.% [5] to 10mol.% [6] of propane. The separation of propane from propylene

is less economical in comparison to the cost of high conversion reactors. Alternative flow schemes include the use of a de-propanizer column for low-purity propylene (60 - 85mol.%) [1].



In the Q-Max cumene production process, the separated DISB and TISB are reacted with a fraction of recovered benzene at optimal conditions for trans-alkylation to produce additional cumene [1]. In a study of the cumene production process [5], the two dominant design optimization features were the alkylation and trans-alkylation reactor size and the benzene recycle stream. An increase in either parameter increased the capital and energy cost; an inverse effect was observed with the number of undesirable by-products in the reactor effluent [5].

The stoichiometry of the alkylation reaction predicts a one-to-one mole ratio of propylene and benzene required for the formation of 1 mole of cumene. However, the benzene to propylene (B:P) ratio in most industrial-scale cumene production processes and patents vary between 2:1 [1] to 7.3:1 [7] [1] [6] [5] [8]; SPA and hydrogen fluoride catalysts require high B:P ratios to maintain competitive cumene yield [1]. The conversion of propylene is also improved at lower B:P ratios by increasing the temperature of the reactor influent; however, selectivity is adversely affected [5]. Selectivity in the previous and following context refers to the amount of cumene formed per mole of propylene when DISB is the only biproduct.

The minimum molar feed ratio required for a preferred single pass yield of cumene is dependent on the selectivity of catalyst to conversion reactions that produce cumene. The maximum cumene yield with SPA is 95% at a minimum 7:1 feed ratio; zeolite-derivative catalyzed processes approach 99.8% yield with a minimum of 2:1 feed ratio [1]. SPA catalyzed cumene production promotes oligomerization of propylene [1] and the formation of poly-isopropylbenzene (PISB) [8]; the latter cannot be trans-alkylated [8]. This factor is commonly cited in the literature [1] [4] for the comparatively lower single-pass yield and overall yield (i.e., including trans-alkylation unit) to zeolite catalyzed processes. Consequently, an excess of benzene is used to minimize olefin oligomerization in the SPA catalyzed process [1]. Zeolite catalysts such as QZ-2500H minimize the rate of olefin oligomerization and are independent of the B:P ratio due to high

selectivity at low temperatures [1]. However, higher temperatures and B:P ratios in zeolite catalyzed processes are also beneficial for higher cumene yields, but the effect is limited [6].

Cumene processes based on zeolites are environmentally friendly [6] alternative and exceptionally stable with catalyst cycles of more than five years [1]. Before 1990, gas-phase-acid-catalyzed alkylation processes were prevalent [6]. However, the most widely used process of cumene production involves the use of zeolite catalysts in a liquid phase reaction; these processes are licensed by Badger LLC, UOP, and Lummus [9].

There were numerous methods of modeling the alkylation and trans-alkylation reactions in the reviewed literature. The most common approach involves the simplification of reactor operation into two main kinetic pathways: the alkylation of propylene and benzene, and the poly-alkylation of propylene and cumene. The products of each are cumene and DISB respectively; in this case, trans-alkylation of DISB and benzene, olefin oligomerization, and hydride transfer reactions are not modeled. Luyben [5] and Vivek et al. [10] applied this modeling methodology with kinetic data derived by Turton et al. [11], displayed in

Table 1. Dimiam et al. [6] used similar kinetic equations with lower magnitude parameters for cumene and DISB formation; trans alkylation was modeled as an equilibrium reaction. Norouzi et al. [8] modeled the alkylation reactor with the same kinetic parameters as Dimiam et al. [6]. They included forward and backward kinetic information for the trans-alkylation of DISB and benzene. Unlike Turton et al. [11], Norouzi et al. [8] and Dimiam et al. [6] modeled both alkylation and poly-alkylation reactions as first order with respect to propylene only; it is shown that the alkylation reaction follows the Eley–Rideal kinetic model, in which propylene adsorption is the rate-determining step [8].

Table 1 below is a summary of reviewed kinetic information for alkylation, poly-alkylation, and trans-alkylation.

Table 1. Summary of Reaction Kinetics for Alkylation, Poly-alkylation and Trans-Alkylation Reactions

Reaction Kinetic Parameters	Alkylation		Poly-alkylation		Trans-alkylation
	Turton et al. [11]	Dimiam et al. [6]	Turton et al. [11]	Dimiam et al. [6]	Norouzi et al. [8]
A	2.8×10^7	6510	2.32×10^9	450	$A = 2.529 \times 10^8$ $A' = 3.877 \times 10^9$
E	104174	52564	146742	55000	$E = 100000$ $E' = 127240$
Rate Equation	$r = Ae^{(-\frac{E}{RT})}C_P C_B$	$r = Ae^{(-\frac{E}{RT})}C_P$	$r = Ae^{(-\frac{E}{RT})}C_P C_B$	$r = Ae^{(-\frac{E}{RT})}C_P$	$r = Ae^{(-\frac{E}{RT})}X_B X_D$ $r' = A'e^{(-\frac{E'}{RT})}X_C^2$
Reaction Phase	Gas	Liquid	Gas	Liquid	Liquid
Pressure Range	25bar	2.5-3.5MPa	25bar	2.5-3.5MPa	-
Temperature Range	300 ⁰ -500 ⁰ C	150 ⁰ -200 ⁰ C [8], 160 ⁰ -220 ⁰ C [6]	300 ⁰ -500 ⁰ C	150 ⁰ -200 ⁰ C [8], 160 ⁰ -220 ⁰ C [6]	220 ⁰ -240 ⁰ C
<ul style="list-style-type: none"> • A', E' and r' refer to kinetics parameters of the reverse reaction • X_B, X_D and X_C are liquid mole fractions • E is in kJ/kmol, rate of reaction is in kmol/m³s • C_P and C_B are concentrations in kmol/m³ 					

2. OBJECTIVES

The objective of this report is the design of two gas-phase alkylation reactor variants that achieve a 95% cumene yield from propylene within design constraints. The constraints include a minimum B/P feed ratio of 5:1, a maximum reactor volume of 20 m³, and a maximum pressure drop of 100 kPa across each reactor. The propylene feed contains a 5 mol.% propane impurity, and the total propylene supplied is 104 kg-mol./h. In addition, each reactor variant is constrained to the utilization of a beta-zeolite derivative catalyst (QZ-2500H) with a density of 2000 kg/m³ and a particle diameter of 1 mm.

The propylene input flowrate of 104 kg-mol./h, at a 95% cumene yield is equivalent to a production rate of 100,000 metric tons of cumene per year. This is consistent with typical annual plant capacities described by Turton et al. [11]. The high B/P ratio was selected because Robert et al. [1] found that an excess benzene input to the reactor minimizes poly-alkylation and olefin oligomerization rates.

The B/P ratio is expressed as the ratio of total benzene to propylene fed into the reaction; a portion of the benzene is supplied from the recycle stream, and the remainder is made up of the fresh feed. The cumene impurity in the recycle benzene stream is assumed to be negligible; cumene does not participate in the primary alkylation reaction and has no foreseeable effect on yield. A sensitivity study of the effect of percentage cumene in the recycle benzene stream will be performed for the overall plant design to determine the validity of the assumption. The block flow diagram in Figure 1 shows the input streams and effluent mole compositions for the desired cumene yield.

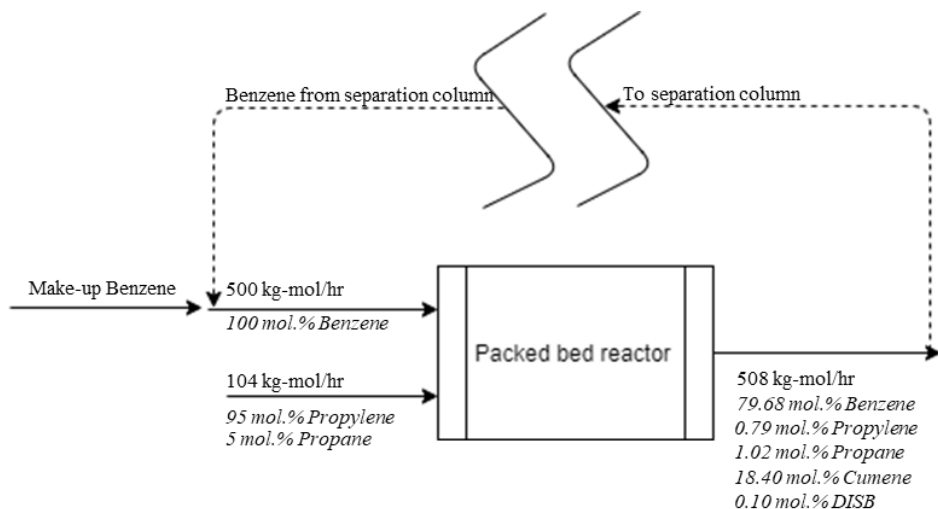


Figure 1. Block flow diagram of the feed and effluent stream of the alkylation unit for a cumene yield of 95%.

In Figure 1, the effluent benzene flowrate of 404.77 kg-mol/h enters a distillation column. Assuming a benzene recovery of 98% at the distillate and a 3:2 split of the recovered benzene is fed between the alkylation and trans-alkylation reactors, respectively. Then, 238 kg-mol/h of benzene is recycled to the alkylation reactor, and a total of 262 kg-mol/h of fresh benzene is feed to the reactor.

2.1. Model Limits and Assumptions

The gas-phase reactors will be modeled in Aspen Hysys as plug flow reactors with the Peng-Robinson fluid package. The Peng-Robinson fluid package was established to accurately predict experimental VLE data of the feed and effluent stream in Report 1. Alkylation and poly-alkylation are the only reactions considered in the alkylation unit, and DISB is the only modeled side product. This is because of the lack of kinetic data for oligomerization side reactions on beta zeolite catalysts in literature. As a result, only the gas phase rate equations for alkylation and poly-alkylation in table 1 will be used to model the alkylation unit.

The total moles of products formed is lower than reactants in the alkylation reaction of benzene and propylene. According to Le Chatelier's principle, higher pressures will favor the yield

of products [5]. The maximum pressure possible for which the available rate equations of alkylation and poly-alkylation are defined is 25 bar. Therefore, an operating pressure of 25 bar was selected for each reactor variant.

The cumene yield of each reactor will be optimized with the manipulation of the total reactor volume, and operational temperature. The inlet temperature into each reactor is constrained to a 500°C maximum, and a minimum temperature of 300°C. The operational temperature upper limit was selected to minimize catalyst deactivation via sintering; the rate of sintering becomes significant at temperatures greater than 500°C [12]. The rate of oligomerization increases at higher temperatures [1]; this adversely affects cumene yield. In addition, 500°C is the upper limit for which the available rate equations in table 1 are defined. A lower limit of 300°C is selected to minimize the risk of condensation of the feed stream; the dew point temperature of the feed mixture is 220°C at 25 bar. The lower temperature limit was also selected because the rate of deactivation of QZ-2500H increases at lower temperatures [1]. Finally, the lower temperature limit of reactor operation was selected because the rate equations for the alkylation and poly-alkylation are undefined below 300°C

2.2. Process Overview and Feed Pre-treatment

Propylene and fresh benzene enter the alkylation circuit as pressurized liquids at 25 bar and 25°C. High pressure is necessary for the propylene feed to remain in the liquid phase because of the relatively high bubble point pressure of 11 bar at 25°C. In contrast, benzene has a comparatively lower bubble point pressure of 0.13 bar at 25 degrees. However, the fresh benzene is pressurized to 25 bar to prevent backflow when mixed with the propylene stream before entering the reactor.

The alkylation reaction occurs in the gas phase. Therefore, the propylene and benzene mixture must be vaporized before reactor entry. The temperature of the mixture is increased to 240°C with a heater; this is 20 degrees above the bubble point temperature at 25 bar. An 8,310kW heater will be required to raise the temperature of the feed mixture by 214 degrees with a pressure drop of 0.3 bar. The 8,310kW heater utilizes steam at 2 bar and 400°C with a flowrate of 8,121kg-mol./h. According to Towler et al. [13], the average heat transfer coefficient for steam-powered vaporizers for light organics is 1050 W/m²K. Therefore, the overall heat transfer area for a vaporizer duty of 8,310kW and LMTD of 193.7°C is 47.35 m².

The benzene and propylene stream leaving the vaporizer has a vapor fraction of 1. The application of an expansion valve on the feed to minimize the heating load was explored. However, the pressure drop required for a vapor fraction of 0.1 at the expansion valve outlet was 24 bar. Figure 2 shows a simplified PFD of the alkylation reactor, including the heating unit.

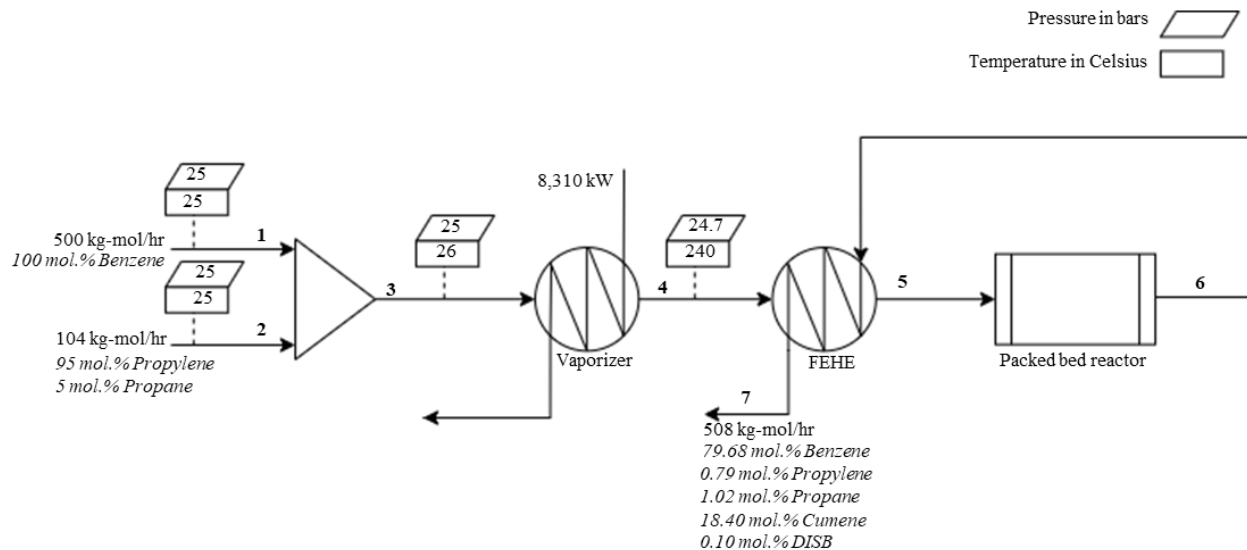


Figure 2. Schematic of typical packed bed reactor design with auxiliary equipment and key stream properties.

Stream 4, in Figure 2, is pre-heated by a Feed Effluent Heat Exchanger (FEHE) to the desired reactor input temperature at stream 5. The energy required to pre-heat the feed stream is derived from the effluent stream, stream 6, of the packed bed reactor. The cooled effluent, stream 7, should have the same composition as the BFD in Figure 1, for the 95% cumene yield constraint.

3. ISOTHERMAL CASE STUDY

An isothermal study of the packed bed reactor was completed with Aspen Hysys. The effluent stream temperature was held constant and equal to the feed temperature while the reactor volume was varied. This was repeated for multiple inlet temperatures between 300°C and 500°C, and the cumene yield was monitored. Figure 3 is a summary of the adiabatic study set-up in Aspen Hysys.

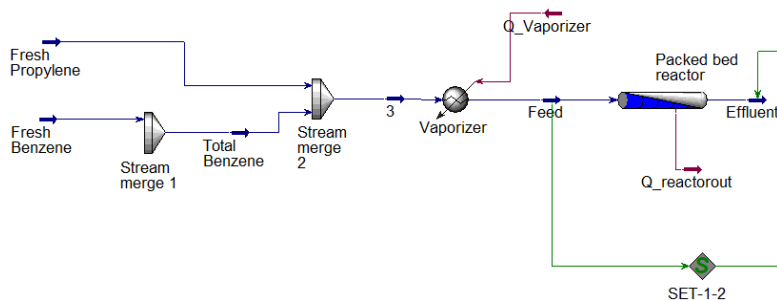


Figure 3. Schematic of isothermal study in Aspen Hysys

In Figure 3, the FEHE is not included in the case study set-up because the vaporizer is sufficient for feed temperature manipulation. Further, the addition of FEHE would interfere with the operation of the set function. The results of the isothermal case study are summarized in Figure 4

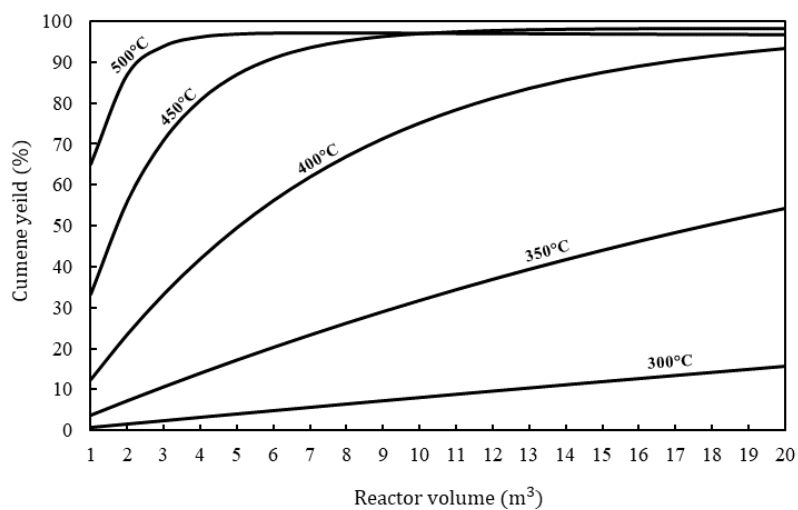


Figure 4. Yield of cumene for isothermal reactor operation as a function of reactor volume at different inlet temperature

According to Figure 4, an increase in the isothermal reactor volume is associated with an increase in cumene yield for a constant feed composition. In addition, an increase in temperature at a constant reactor volume the cumene yield of an isothermal reactor; therefore, the higher feed temperatures achieve can achieve the desired yield with lower reactor volumes. An isothermal reactor with a feed temperature greater than 400°C can achieve the desired yield of 95% with reactor volume less than 20 m³.

4. ADIABATIC CASE STUDY

An adiabatic reactor case study of cumene yield as a function of reactor volumes, at multiple feed temperatures, showed similar trends to the isothermal study. The case study set up, in Figure 5, involved the removal of the deactivation of the set function, and the removal of the energy stream from the packed bed reactor. The adiabatic and isothermal case studies were evaluated with equal feed compositions and flowrates. The results of the adiabatic case study are shown in Figure 6.

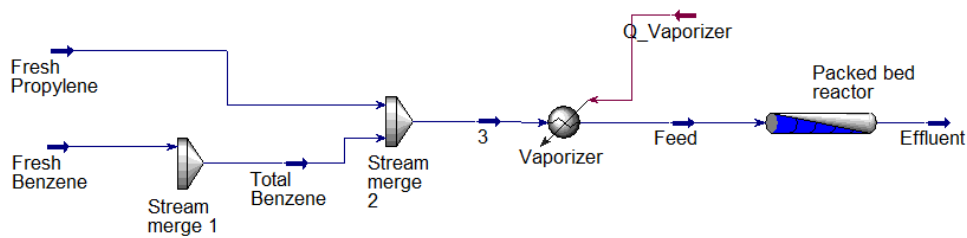


Figure 5. Schematic of adiabatic study in Aspen Hysys

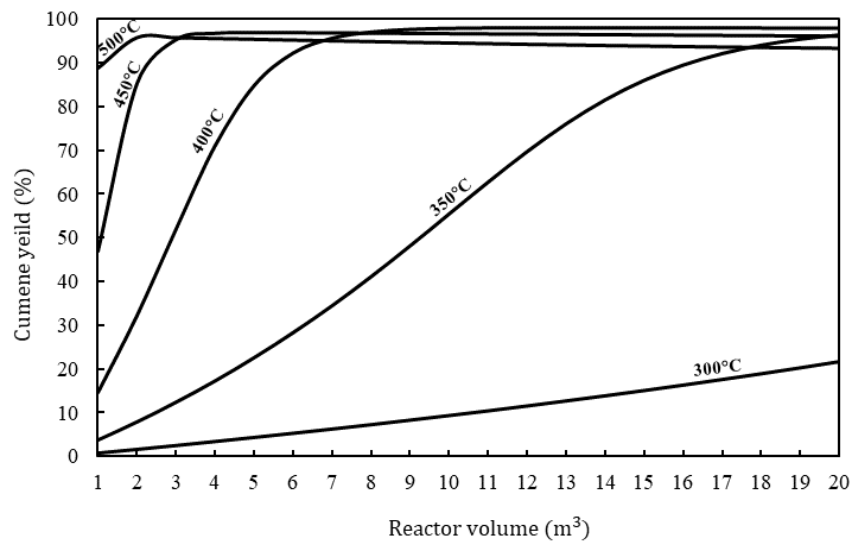


Figure 6. Yield of cumene for adiabatic reactor operation as a function of reactor volume at different inlet temperature

According to Figure 6, an increase in the volume of an adiabatic reactor is associated with higher cumene yields for a constant feed temperature. In addition, higher feed temperatures at a constant volume result in greater cumene yields. However, adiabatic reactors achieve higher yields compared to isothermal reactors when normalized feed temperatures and operational volumes. An adiabatic reactor can achieve the desired yield of 95% at feed temperatures greater or equal to 350°C and volumes less or equal to 20 m³. This is likely due to the exothermic nature of the alkylation reaction; the energy released increases temperature, the rate of reaction, and propylene conversion for a fixed volume. Figure 7 shows the results of a study of the effluent temperature of an adiabatic reactor as a function of volume for different feed temperatures.

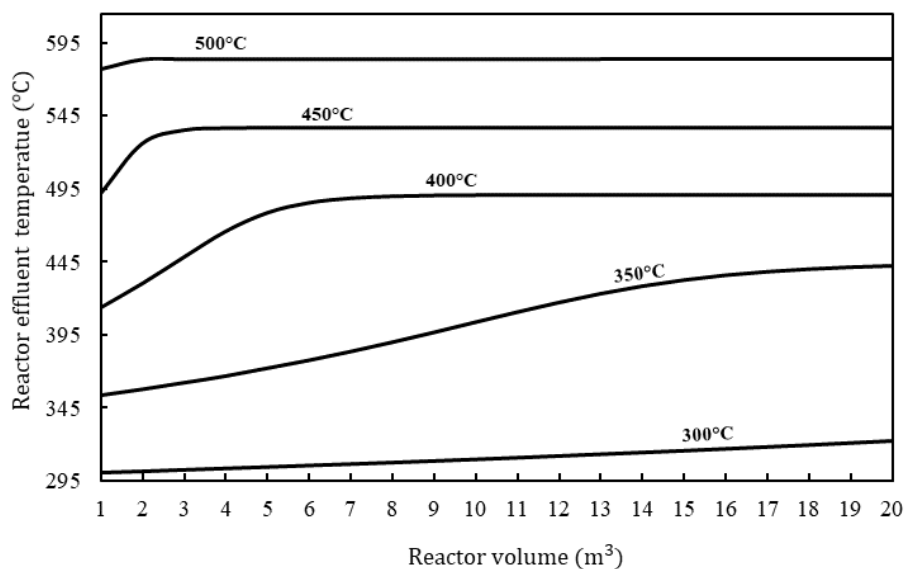


Figure 7. Outlet temperature for adiabatic operation as a function of reactor volume for various inlet temperature

From Figure 7, the effluent temperature increases as a function of the volume in an adiabatic reactor. Although the feed temperature of the reactor may be within limits, Figure 7 shows that the outlet temperature may exceed the upper limit of the temperature constraints at specific reactor volumes. A feed temperature equal to 450°C will result in outlet temperatures exceeding 500 degrees for all reactor volumes in the considered range. However, feed temperatures between 350°C to 400°C will result in outlet temperatures below 500°C for all considered reactor volumes.

Also, Figure 6 shows that a 20 m³ adiabatic reactor would be required for a 95% cumene yield when the feed temperature is 350°C; conversely, 7 m³ is required at a feed temperature is 400°C

The feed temperature of an adiabatic reactor may be increased beyond 400°C for a fixed range of volumes before cooling is required to prevent catalyst deactivation. Figure 8 shows the effluent temperature as a function of reactor volume, for 10°C increments above a feed temperature of 400°C

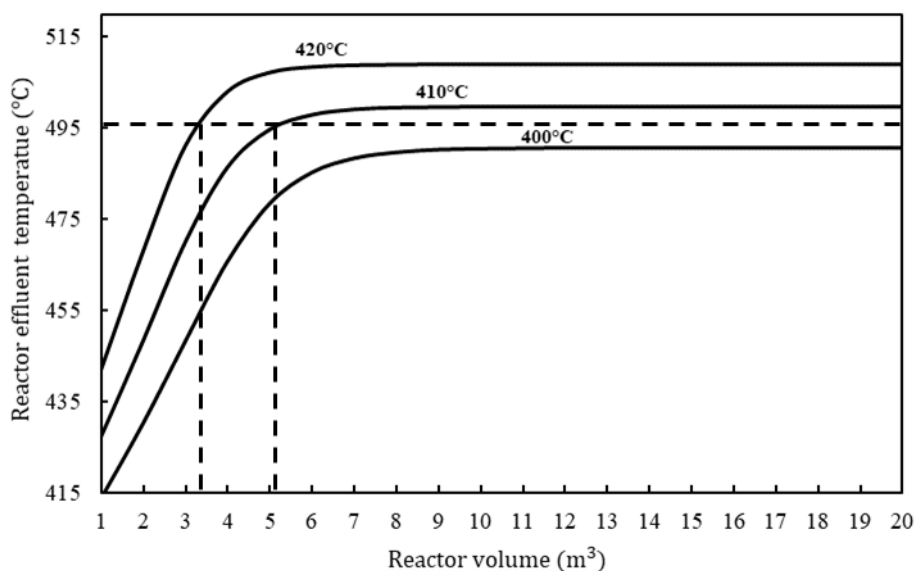


Figure 8. Outlet temperature for adiabatic operation as a function of reactor volume for inlet temperatures of 400°C, 410°C, and 420°C.

Figure 8 shows that the maximum allowable reactor volume required for the maintenance of an outlet temperature below 500°C is reduced as the feed temperature increases. The maximum allowable volume for feed temperatures of 410°C and 420°C is 5.1 m³ and 3.2 m³, respectively. Figure 9 shows the cumene yield as a function of volume at feed temperatures marginally greater than 400°C

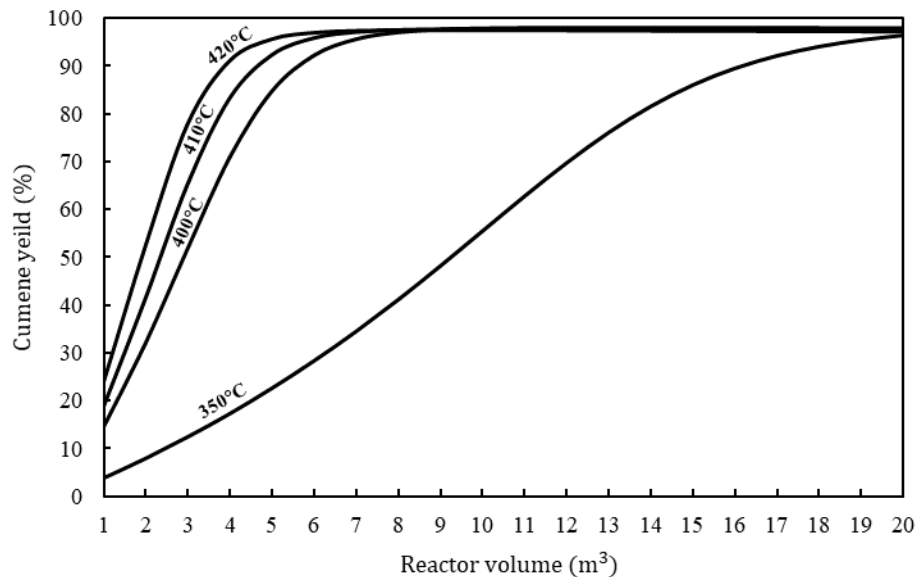


Figure 9. Yield of cumene for adiabatic reactor operation as a function of reactor volume at inlet temperatures of 400°C, 410°C, and 420°C

In Figure 9, the yield at the maximum allowable adiabatic reactor volume, for feed temperatures of 410°C and 420°C, is 91% and 80%, respectively. Therefore, more than one adiabatic reactor in series is required to achieve the desired cumene yield for feed temperatures higher than 400°C. Also, inter-stage cooling is required to minimize the temperatures of streams between reactors to avoid catalyst deactivation and higher oligomerization rates.

5. REACTOR DESIGN

A variant of the packed bed reactor will be designed as a low-temperature adiabatic PFR unit and the other as high-temperature inter-stage cooled adiabatic PFR reactors. Both reactors will be designed to each achieve a 95% cumene yield for the same feedstock shown in Figure 1. The selected reactor volumes for high feed temperatures (i.e., 410°C or 420°C) will be less than the maximum allowable volume to minimize the effluent temperature reasonably below 500°C. This will also reduce the expected cumene yield per reactor below 91% and 80% for 410°C, and 420°C feed temperatures, respectively.

5.1. Reaction Variant One

The adiabatic study in Figure 6 shows that a feed temperature of 350°C will require a total volume of approximately 20 m³ to achieve a 95% cumene yield. Figure 7 shows that the maximum effluent temperature for a 20 m³ adiabatic reactor with a feed temperature of 350°C, is 442°C. Therefore, the first packed bed reactor variant features a low-temperature input stream of 350°C and a total reactor volume of 20 m³. The reactor should be constructed with carbon steel [1] and contain 10 tubes, each with a diameter of 0.6212 m and a length of 6.6 m. The calculated pressure drop across the reactor for a void fraction of 0.5 and a catalyst diameter of 1 mm, is approximately 0.23 bar. The feed is pre-heated from 240°C to 350°C with a TEMA type-AFU feed-effluent heat exchanger (FEHE). The detailed heat exchanger dimensions are shown in Table 2.

Table 2. Summary Feed Effluent Heat Exchanger Sizing Parameters for Reactor Variant One

Parameter	Value
Tube Inlet Temperature	442.5°C
Tube Outlet Temperature	342.4°C
Shell Inlet Temperature	240.0°C
Shell Outlet Temperature	350.0°C
Tube OD	20.00 mm
Number of Tubes	150
Tube Length	6 m
Shell Diameter	716 mm
Shell volume per Shell	2.136 m ³
Overall UA	1.052×10^5 kJ/°C-h
Average Heat Transfer Coefficient (gas-gas shell and tube) [13]	30W/m ² K
Transfer Area	972 m ²

The reactor effluent enters the tube side of the FEHE while the feed enters the shell side in counter-current flow. There are two tube passes in the FEHE as a result of the U-tube rear end, and two shell passes separated by a longitudinal baffle. The preliminary heat exchanger dimensions are shown in table 1. Figure 10 shows the PFD of the first reactor variant

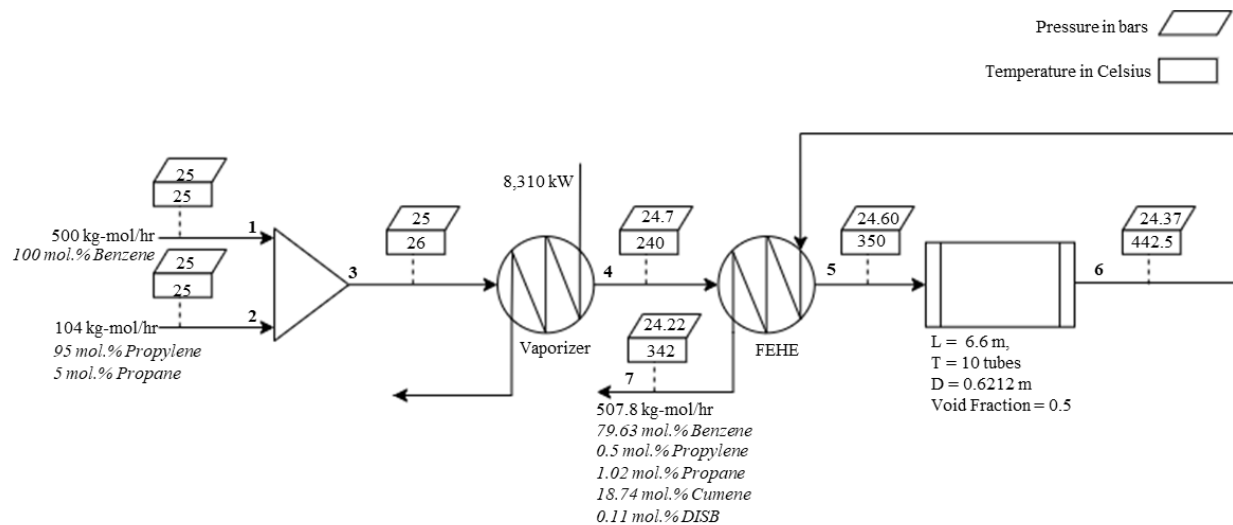


Figure 10. PFD of reactor variant one with effluent stream composition with stream pressures and temperatures

In Figure 10, the reactor effluent contains 95.16 kg-mol./h of cumene; equivalent to 96.3% cumene yield from propylene. There is a 96.85% conversion of propylene for the alkylation reaction and an overall propylene conversion of 97.4% in the reactor. The main control loops for the reactor system are shown in Figure 11

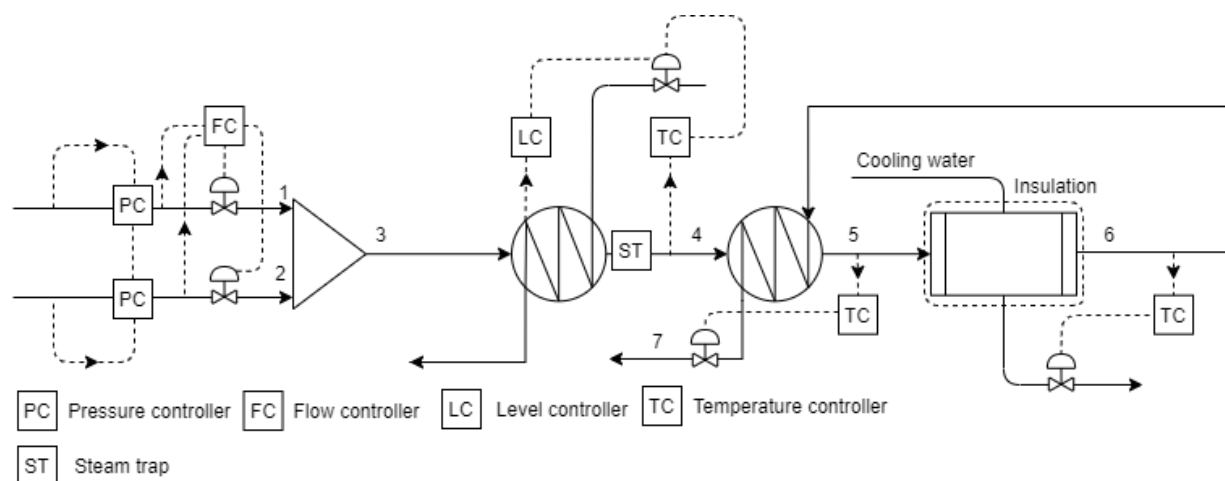


Figure 11. P&ID diagram of first reactor variant showing primary control loops

In Figure 11, the pressure of stream 1 and 2 are controlled with a pressure control system that manipulates power supplied to the propylene and benzene feed pumps. The flow controller maintains the B/P feed ratio in stream 3 at the desired set-point with the manipulation of the valves on the stream 1 and 2. The level controller is a safety feature in the vaporizer system, which prevents liquid overflow. The liquid height in the vaporizer is controlled with the manipulation flowrate of steam to the vaporizer system. The effluent stream of the vaporizer may contain some condensate before entering FEHE due to heat losses to the environment. A modified stream trap at the FEHE inlet, in-stream 4, removes and re-recycles condensate back to the vaporizer. This minimizes the required total energy required to raise the feed temperature to the desired temperature at the FEHE. The temperature controller on stream 4 manipulates the power supplied to the vaporizer to control the temperature. The temperature of stream 5 is controlled with the manipulation of flowrate of the cooled reactor effluent stream exiting the FEHE. In this reactor design, the effluent temperature is expected not to exceed 500°C or drop below 442°C. However,

heat losses to the environment can cause cooling, and input temperatures greater than 400°C cause effluent temperatures greater than 500°C.

Heat losses can be minimized with the installation of insulation. A safety measure against high-temperature outputs is the installation of a cooling jacket underneath the insulation. The reactor effluent temperature, in stream 6, is monitored and controlled with the manipulation of the cooling water flowrate over the reactor.

5.2. Reactor Variant Two

According to Figure 8, multiple adiabatic reactors in series are required to achieve the desired cumene yield for feed temperatures higher than 400°C. The maximum reactor volume allowable for a feed temperature of 420°C is 3.2 m³, with a cumene yield of 80%. A lower feed temperature of 410°C has a higher maximum volume allowable of 5.2 m³ and a higher cumene yield of 91%. However, the cumene yield was evaluated at the maximum allowable volume. At equal reactor volumes lower the 3.2 m³, a feed temperature of 420°C consistently results in higher yields compared to a feed at 410°C. Therefore, a feed temperature of 420°C was selected for the second reactor variant because reactor volume is conserved, and results in higher cumene yields relative to lower temperatures. However, inter-stage cooling will be required to reduce the temperature of the stream between reactors within temperature constraints.

The second reactor variant is modeled as 3 adiabatic reactors in series, each with a volume of 2 m³, 3m³, and 5.5m³, respectively. There are inter-stage coolers between the first and last two reactors. The length, diameter, and the number of tubes of each reactor are shown in Figure 12. There is a pressure drop of 0.38, 0.14, and 0.22 bar across the first, second, and third reactors, respectively. All reactors utilize a beta zeolite catalyst with a 1mm particle size. The first two reactors have a void fraction of 0.5, and the third has a void fraction of 0.6.

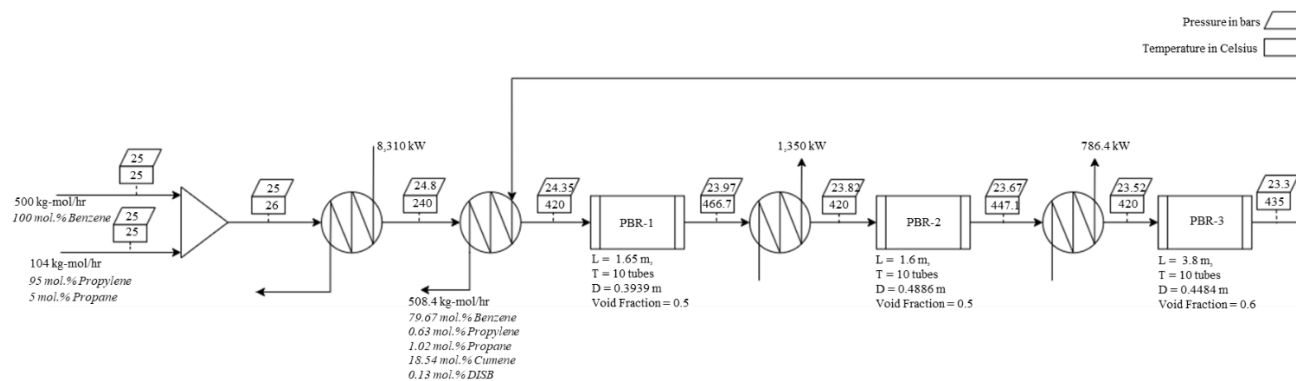


Figure 12. PFD of reactor variant two with effluent stream composition with stream pressures and temperatures

Each inter-stage cooler has a tube-side pressure drop of 0.15 bar and cools the effluent previous PBR stage to 420°C. In Figure 12, the 1350kW and 786.4kW coolers utilize cooling water at 25°C with flowrates of 1830 kg/h, and 1073kg/h, respectively. The preliminary sizing parameters for the auxiliary equipment is shown in Table 3.

Table 3. List of Auxiliary Equipment and Utilities in Reactor Variant Two

Unit	Purpose	Utility	Duty	LMTD	Average Heat Transfer Coefficient	Heat Transfer Area	Material
8310kW vaporizer	Reactor feed vaporizer	Steam, 2bar, 400°C	2.990×10^7 kJ/°C-h	167.4°C	1050 W/m ² K (steam heating light organics) [13]	47.35 m ²	Carbon steel
1350kW cooler	PBR-1 effluent cooler	Water, 2bar 25°C	4.825×10^6 kJ/°C-h	368.0°C	160 W/m ² K (water cooling light organics coolers) [13]	227.43 m ²	Carbon steel
786.4kW cooler	PBR-2 effluent cooler	Water, 2bar 25°C	2.83×10^6 kJ/°C-h	368.0°C	160 W/m ² K (water cooling light organics) [13]	13.70 m ²	Carbon steel

The third reactor has a volume higher than the maximum allowable for an input temperature of 420°C. This is because 80% of the propylene is fed to PBR-1 has been consumed before entering PBR-3. Therefore, the heat released and temperature rise due to the alkylation reaction is lower in the third reactor. In Figure 12, the effluent of the third reactor contains 94.2 kg-mol./h of cumene; There is a 95.3 % overall cumene yield from propylene for all 3 reactors, and a 94.7% overall propylene conversion. The feed stream is pre-heated by the effluent of the final reactor with a TEMA type-AFU FEHE in the same orientation as the first reactor variant. The preliminary sizing details of the heat exchanger are shown in Table 4.

Table 4. Summary Feed Effluent Heat Exchanger Sizing Parameters for Reactor Variant Two

Parameter	Value
Tube Inlet Temperature	435.0°C
Tube Outlet Temperature	261.3°C
Shell Inlet Temperature	240.0°C
Shell Outlet Temperature	420.0°C
Tube OD	20.00 mm
Number of tubes	74
Tube length	6 m
Shell diameter	510.7 mm
Shell volume per Shell	1.090 m ³
Overall UA	1.03×10^6 kJ/°C-h
Average Heat Transfer Coefficient (gas-gas, shell and tube) [13]	30 W/m ² K
Transfer area	9500 m ²

The main control loops for feed pre-treatment in the second reactor variant are the same as those of the first reactor variant. However, there are additional control loops for the control of the temperature of each cooler effluent stream. In this case, the stream temperature is controlled with the manipulation of the cooling water flow rate through the heat exchanger. Figure 13 shows the main control loops for the second reactor variant

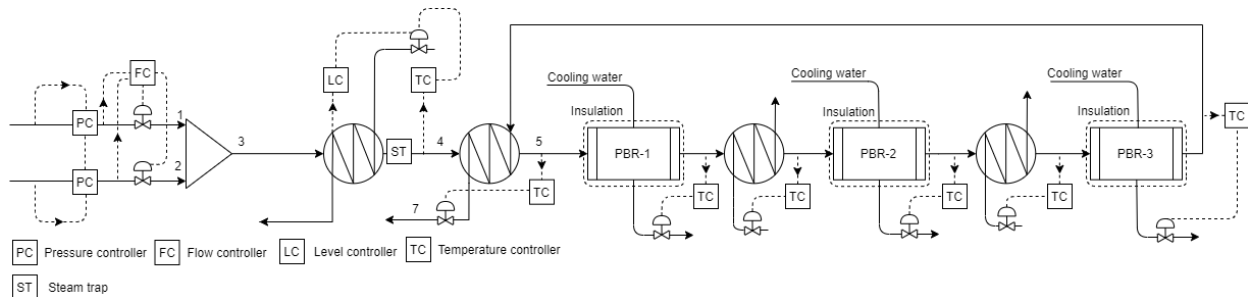


Figure 13. P&ID diagram of second reactor variant showing major control loops

6. ECONOMIC ANALYSIS

The economic analysis of each reactor system was completed with a capital cost estimation tool called Cap cost. The cost of raw material was obtained from different years, and are not consistent with present raw material prices. This could cause overestimation or underestimation of operational costs in reference to current prices. The cost of all equipment and associated utilities are summarized in Table 5.

Table 5. Summary of Capital and Operational Costs for Variant One and Two

Equipment	Capital costs (module cost)		Utility	Annual operational costs	
	Reactor Variant One	Reactor Variant Two		Reactor Variant One	Reactor Variant Two
8310kW vaporizer	\$ 63,700	\$ 63,700	Steam, 2bar, 400°C	\$ 505,000	\$ 505,000
1350kW cooler	–	\$ 400,000	Water, 2bar, 25°C	–	\$ 191,500
786.4kW cooler	–	\$ 26,209	Water, 2bar, 25°C	–	\$ 112,300
FEHE	\$1,763,026	\$ 24,600,000	Reactor Effluent	–	–
Packed bed reactors	\$17,100,000	\$ 16, 990,000	Benzene supply at price of \$0.876./kg [14]	\$ 149,154,873	\$ 149,154,873
			Propylene supply at price of \$0.97/kg [8]	\$ 33,560,754	\$ 33,560,754
Zeolite catalyst at a price of \$10/kg [14]	\$ 200,000	\$ 94,000	–	–	–
Total	\$19,126,726	\$25,183,909		\$183,220,627	\$183,524,427

The second reactor variant minimizes capital costs as a result of lower reactor volume and catalyst requirements. However, the addition of inter-stage coolers and a larger FEHE transfer area increases the capital cost by \$6,057,183 above the first reactor variant. The first reactor variant has an operating cost of \$303,800 lower than the second reactor variant due to the additional cooling requirements of the second variant. Both reactor variants produce approximately 11250.5 kg/h of

cumene. The annualized credit from cumene at a selling price of \$1.47/kg [15] is \$137,351,594 for both reactors. The total annualized operating costs of the first reactor variant is \$45,589,925 greater than the credit from cumene sold; the operating costs are \$46,172,833 greater for the second variant.

At a minimum, there is no profit made from the balance between the cost of reactants and credits from cumene yield for both reactors. This is still the case for a production rate of 11,880kg/h of cumene (100% cumene yield from propylene). However, fresh benzene fed at 350 kg-mol/h and propylene at 261 kg-mol/h, at 98% cumene yield would result in a positive annual margin of \$88,628,603 between cumene sales and benzene and propylene cost. The next steps would involve the redesign of the previous reactor variants with more economic molar feed ratios, and higher minimum cumene yields.

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