

Design Report for the Production of Cumene

Submitted to:

Dr. John Schlup

CHE 570

Submitted by:

Tristan Grieves, Nikki Klaassen, Patrick O'Connor, Sarah Keffer

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Executive Summary

This design report outlines an isopropylbenzene, or cumene, production facility with a process flow diagram, sized equipment, and an economic analysis of the process. The facility uses a preheater and a fired heater to increase the temperature of the feed to reactor conditions. The reactor is a packed bed reactor, packed with 30% proprietary catalyst and 70% inert packing. The product stream is separated using three distillation columns. The first column separates the propane impurity and the recycle stream from the sellable product streams. The second column separates the impurity to be used as a fuel gas from the recycle. The final column separates the two products, cumene and diisopropylbenzene, into the required purities to sell.

The facility is designed to produce 96.2 thousand tonnes of cumene annually, at a purity of 99.5 mol%. The facility also produces 3.74 thousand tonnes of diisopropylbenzene with a purity of 98.6% as a byproduct that can also be sold. The propane impurity from the propylene feed is used as a fuel gas, reducing the amount of fuel gas needed to be purchased.

The process has a capital cost of \$29.4 million over the two years of construction, with a fixed capital investment of \$25 million, and a working capital of \$4.4 million. The process has a discounted payback period of 4 years after startup. The process has a net present value of \$27.8 million at a minimum rate of return of 15%.

The process was simulated using Aspen Plus V8.8, while PolyMath was used for initial reactor designs. The economics were calculated using the guidelines from *Analysis, Synthesis, and Design of Chemical Processes* by Turton, Bailie and Whiting, and equipment costs were calculated using the CapCost spreadsheet provided with the textbook.

The recommended actions derived from this report is that the plant should be approved to move to the next stage of design. Before construction can begin, a more detailed design should be conducted, including a piping and instrument diagram for the full process, and vendor priced equipment. The current model is highly profitable with a quick payback period, and has accounted for differences in expected and actual costs. Further development into this plant will be a valuable investment for the future of the company.

Problem Introduction

Isopropylbenzene, or cumene, is traditionally a key component in global phenol production. With a 2011 market demand of 12.4 million tons (Stephan 2013), this makes cumene production nearly a 20 billion dollar per year industry. Nearly all of the cumene produced in the world uses the reactants benzene and propylene operated at high temperature and pressure over a zeolite (or other) catalyst (Deng-Yang Jan 2013). The Research and Design department at Wildcat Petrochemicals, Inc. has recently developed a new proprietary catalyst. With the proprietary catalyst, Wildcat Petrochemicals, Inc. will attempt place a stake in the global cumene market by providing a more pure product at a similar price. This report will investigate the chemical and economic feasibility of developing a new cumene production process an existing plant site for the synthesis and purification of cumene with an output goal of 100,000 metric tons per year for a plant life of 15 years.

Cumene in the global petrochemical industry is used primarily as a reactant for production of phenol. Benzene and propylene, the two reactants used to create cumene, are produced primarily as a byproduct of crude oil refining. On the downstream side of cumene production, phenol is used to produce important chemicals including bisphenol-A (BPA), polycarbonate resin, and phenolic resins. These chemicals are used extensively in the packaging, construction, and pharmaceutical industries and are expected to increase in demand (Stephan 2013).

The reaction process for the synthesis of cumene involves the Friedel-Crafts alkylation of benzene with propylene as shown in Figure 1. This process typically involves temperatures greater than 350 °C and 30 bar. The primary (and only) byproduct of this reaction as the result of further alkylation of cumene is p-diisopropylbenzene (DIPB), the structure of which is shown in Figure 2. While this product can be if pure, the desirable product for this plant is cumene. This process is assumed to be an irreversible reaction due to a relatively insignificant rate of reverse reaction due to the catalyst and operational temperatures. The catalyst used to increase selectivity towards cumene in the market today is zeolite, a crystalline-aluminosilicate composite. Newer exotic composites involving mixtures of zeolites, inorganic oxides, and silanol are making ground in providing greater selectivity (Deng-Yang Jan 2013). The catalyst developed by Wildcat Petrochemicals, Inc. also shows promise in providing enhanced kinetics at a lower cost.

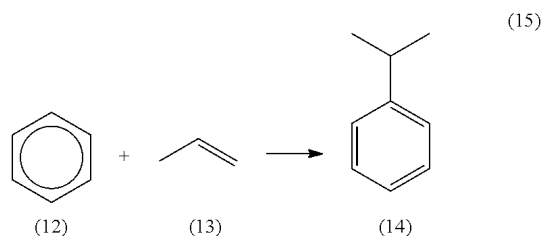
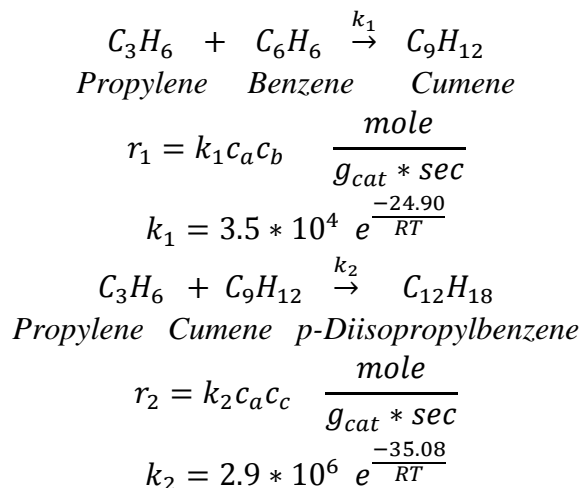


Figure 1. The production of cumene (right) from benzene (left) and propylene (middle). This reaction proceeds irreversibly by Friedel-Crafts alkylation (Deng-Yang Jan 2013).



Figure 2. Structure of *p*-diisopropylbenzene (DIPB). The addition of cumene to propylene via further alkylation leads to this undesired byproduct (NIST 2011).

While the exact structure and chemical composition of the proprietary catalyst remains largely undisclosed, the following reactions and kinetics were provided:



Global market analysis by Wildcat Market Research Solutions, Wildcat Petrochemical's sister company, indicates this is an optimal time to be involved in the production of cumene. The global market of cumene is expected to grow to nearly 50% by year 2020 to an estimated demand of 18 million tons per year. The economic driving force behind this large increase is due to an expected increase in demand from growing industries in Asian-Pacific countries such as China. Even greater demand could be possible in the coming years with expansions being made in phenol production sites such as India (Stephan 2013). Generally, the outlook for cumene demand looks positive.

The current trends in market costs for the reactants, benzene and propylene, also appears to be optimal for entering the cumene production market. Since benzene and propylene are produced as a byproduct from refining crude oil, the prices are directly responsive to crude oil prices. As of 2015, trends in the crude oil prices have taken a dramatic downturn. As a result, benzene and propylene prices have dropped as well. The ICIS Petrochemical Index (IPEX), a measure of global petrochemical prices, shows a dramatic decrease in the 2015 calendar year. With no dramatic raise to pre-2015 crude oil price expected out of OPEC in sight, the low prices of benzene and propylene are expected to stay (ICIS 2015).

A full economic evaluation will be included in the report for an existing plant with new equipment. The project will be built over 2 years and have a project life of 15 years. A

depreciation schedule using MACRS over a 5 year recovery period will be used. All costs will be given in 2013 dollars. A minimal acceptable rate of return is set at 15% per year, with a marginal taxation rate of 35%. A full evaluation of profitability will also be discussed.

While overall outlook looks positive, there are a few concerns for the outlook of cumene demand and production in the market highlighted by Wildcat Market Research Solutions. The global demand for bisphenol-A, an important end-product of phenol, appears to be decreasing in the near future. The main cause for this is that bisphenol-A is currently being phased out of industries that supply human needs because of certain carcinogenic properties (NIEHS 2015). However, this is not the only use for bisphenol-A, and bisphenol-A is only a small part of phenol end-products, so the effect on cumene prices should be minimal. Additionally, great strides are being made in developing process to produce phenol that skip the production of cumene entirely. One such process involves the direct air oxidation of benzene over a copper-chromium catalyst with high selectivity towards phenol (ACS 2014). While this process appears inexpensive in terms of phenol production, it is still far from application in the global industry. In addition, the reaction run time takes roughly 2 hours, which is much slower than current cumene production methods. Overall, opportunity for entrance into the cumene production market is ideal.

The primary health and safety concerns in the process involve primarily the high pressure and temperature streams feeding into and out of the reactor. All products and reactants in this process are flammable if a leak were to occur in the process. None of the products and reactants, nor the coolants used are directly toxic or harmful to humans. A general hazard of operations risk analysis of each piece of equipment will be included in this report. In designing the reactor and separators, great care will be taken in ensuring the safety of those operating the equipment. While the reactants and products used can be harmful to the ozone, any waste generated in this process is expected to be used as fuel for a fired heater.

Results

The final design for cumene production was simulated using Aspen Plus simulation software. A process flow diagram (PFD) of the final process is shown in Figure 3, below. A detailed description of the design can be read in the Process Description section of this report.

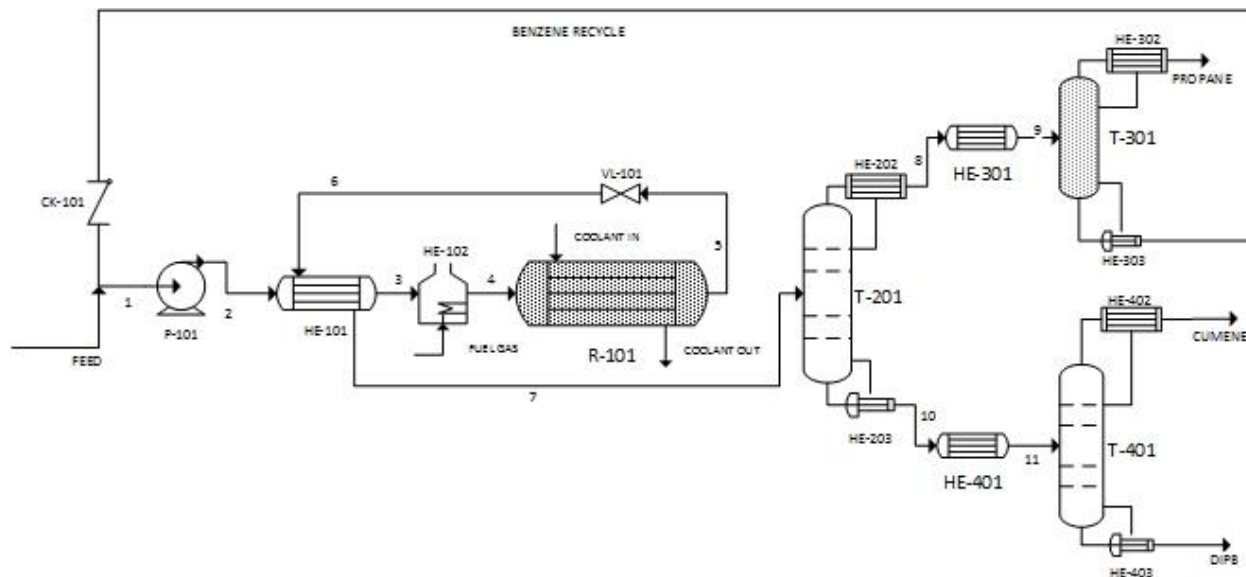


Figure 3. The above figure shows a detailed process flow diagram (PFD) for the cumene production process. Major pieces of equipment are labeled and the general flow can be visualized. The designation P (i.e., P-101) indicates a pump. VL indicates a valve. R indicates a reactor. T indicates a distillation column. HE indicates heat exchanger. All flow streams to and from external sources and recycle are labeled with a name (i.e., FEED), and all subsequent internal streams are labeled with a number (i.e., 9).

The final process used a plug flow reactor to produce the cumene from the reactants, benzene and propylene. DIPB was produced as a byproduct. Three separate distillation columns were employed in order to purify cumene from the byproduct, remaining reactants, and inert (propane). The first column, T-201, separates benzene and propane from the remaining components. The distillate is fed into T-301 to separate benzene from propane, where benzene is recycled back through the reactor. The bottoms of T-201 feed into T-301 where cumene is purified from DIPB.

Table 1 presents the component molar flow rates, temperature, pressure, and vapor quality of streams leaving or entering the process. These are the named streams in the PFD. The required cumene purity for this process was deemed to be 99.5%. The cumene stream contains cumene at 99.5 mol%, matching the minimum required purity of cumene. The DIPB purity in the DIPB stream is 98.6 mol%. This exceeds the requirement of 98% purity of DIPB necessary to sell it as a product. The recycle stream contains benzene and cumene. These are recycled back into the process so as not to waste those resources.

Table 1. The below table shows all name-labeled stream specifications including molar flow rates, temperature, vapor quality, and pressure for the PFD shown in Figure 3. All flow rates are in kmol/hr. All temperatures are in °C. All pressures are in bar.

STREAM	FEED	CUMENE	DIPB	PROPANE	BENZENE RECYCLE	COOLANT IN	COOLANT OUT
Cumene	-	97.30	0.04	-	0.18	-	-
Benzene	102.20	0.43	-	1.60	4.82	-	-
DIPB	-	0.05	2.78	-	-	-	-
Propane	5.03	-	-	5.03	-	-	-
Propylene	103.00	-	-	-	-	-	-
Water	-	-	-	-	-	584	584
Total Flow	210.23	97.78	2.82	6.63	5.00	584	584
Temperature	25	236.4	303.7	92	152.9	20	102.1
Pressure (bar)	1.01	6	6.02	6	6	1	1
Quality	0	1	0	1	0	0	0.275

Table 2, below, presents the component molar flow rates, temperature, pressure, and vapor quality of streams traveling between pieces of equipment. The overall mass balance for each stream is maintained throughout the process. The temperatures and pressures of each stream correspond to the conditions of the piece of equipment it just exited.

Table 2. The below table shows all number-labeled internal stream specifications including molar flow rates, temperature, vapor quality, and pressure for the PFD shown in Figure 3. All flow rates are in kmol/hr. All temperatures are in °C. All pressures are in bar.

STREAM	1	2	3	4	5	6	7	8	9	10	11
Cumene	0.18	0.18	0.18	0.18	97.52	97.52	97.52	0.18	0.18	97.34	97.34
Benzene	107.02	107.02	107.02	107.02	6.85	6.85	6.85	6.42	6.42	0.43	0.43
DIPB					2.83	2.83	2.83			2.83	2.83
Propane	5.03	5.03	5.03	5.03	5.03	5.03	5.03	5.03	5.03		
Propylene	103.00	103.00	103.00	103.00							
Total Flow	215.23	215.23	215.23	215.23	112.23	112.23	112.23	11.63	11.63	100.60	100.60
Temperature	28.9	33.1	211.2	377.2	372	332.9	180	130.5	80	237.3	200
Pressure	1.01	40.5	40.5	40	39.3	6.17	6.17	6	6	6.02	6
Quality	0	0	1	1	1	1	0	1	0.42	0	0

Process Description

Design Goals and Constraints

The main basis of this project for Wildcat Petrochemicals, Inc. is to use the new catalyst properties to develop a reactor and subsequent support systems to produce 100,000 metric tons per year of a 99.5 mol% cumene product for a 15 year plant lifetime with 2 years of construction. The input of benzene is assumed to be pure, while the input of propylene has a 5 mol% impurity of propane. As a byproduct, DIPB can be sold if purity is greater than 98 mol%. The production goal translates to an approximate reactor output of 95 kmol/hr of cumene. Every aspect of the reactor, separation systems, and other units were designed to reach this output goal while minimizing costs, reducing environmental impact, complying with common industry “good practice” standards. These standards are incorporated throughout the design process, and are explained in detail in subsequent sections.

Overall Process Design Description

The final cumene process design is shown as a PFD in Figure 3. The properties and flow rates of each stream of the process can be found in Table 2. At the start of the process, a feed carrying benzene, propane, and propylene (see Table 1 for component flow rates) enters the plant from the storage facility. The Recycle stream intersects the Feed stream at a check valve, VL-101.

Upon mixing the Feed and Recycle streams, Stream 1 enters the first pump, P-101. The pump increases the pressure of Stream 1 from 1.01 bar to 40.50 bar so that the mixture is at reactor operating pressure. This requires a net work of 39.09 kW while operating at a pump efficiency of 50.45 mol%. The pump also increases the temperature from 29°C in Stream 1 to 33°C in Stream 2.

Stream 2 exits the pump and enters the first of two heat exchangers, HE-101. HE-101 is a preheater for the reactor feed stream, while also acting as a condenser for the reactor exit stream. The streams run countercurrent, to allow for a higher heat transfer over the length of the reactor. Stream 3 exits HE-101 at a new temperature of 211°C and enters HE-102, while Stream 7 exits the exchanger at 180°C. HE-102 is a fired heater, with a steady state heat duty of 1434 kW. The fired heater raises the stream to reactor conditions, of 377°C and 40 bar. The pressure drop over both heat exchangers is 0.5 bar.

Stream 4 then exits HE-102 and enters the reactor, R-101. The reactor feed contains large quantities of propylene and benzene, and smaller quantities of propane and cumene, from the feed impurity and the recycle stream, respectively. The reactor operating conditions can be found in the section Reactor Process Overview, and a more detailed description can be found in Appendix A. Stream 5 leaving R-101 contains 86.9 mol% cumene. It also contains small amounts of benzene, and DIPB, and the propane impurity. All of the propylene was consumed in the reactor. Stream 5 exits at as a vapor at a temperature of 372°C and 39.3 bar.

Stream 5 then enters an expansion valve, VL-102. This valve lowers the pressure of the stream to 6.17 bar for a pressure drop of 33.1 bar while decreasing the temperature to 332°C. Stream 6 then exits the valve and enters H-101 as the hot shell-side fluid. This allows energy already in the system to be used to preheat the feed stream while condensing the reactor outlet stream. This cools the stream to an exit temperature of 180°C.

Stream 7 exits HE-101 and enters the first distillation tower, T-201. Operating conditions of each tower can be found below in the section Separation Process Overview, and a more detailed description can be found in Appendix B. T-201 is designed so that benzene is the light key, and cumene the heavy key. This separation allows for a small column for the distillate to separate the recycle, and a secondary large column to separate out the DIPB.

The distillate of this column, Stream TOP1, contains 55.2 mol% benzene, 43.3 mol% propane and a small cumene impurity. Stream TOP1 then enters a heat exchanger, HE-103 to prepare the stream for the second tower. HE-103 lowers the stream temperature from 130.5 to 80°C while operating at 6 bar, with a net heat duty of 69 kW. Stream 8 leaves HE-301 as a liquid and enters T-301, the second distillation tower. This tower is designed to remove the propane from the recycle stream. The distillate stream, Propane, exits the column with 75.9 mol% propane and the remaining molar flow consisting of benzene. The stream exits at 6 bar and 92°C. The bottoms stream of T-301 is the Recycle stream. This stream contains 96.4 mol% benzene with the remaining molar flow consisting of cumene. This stream exits at 6 bar and 153°C and is transported back to the start to add into the initial Feed stream.

The bottoms stream of T-201, BOT1, exits the reactor at 237°C. It contains 96.75 mol% cumene, 2.8 mol% DIPB, and the remaining molar flow is made up of benzene. BOT1 enters a heat exchanger, HE-104, to lower the temperature. HE-104 has a net duty of 320 kW and lowers the temperature from 237°C to 200°C in Stream 9. Stream 9 is then ready to enter the third distillation tower, T-401.

T-401 separates cumene and the remaining benzene from DIPB. The distillate stream, CUMENE, exits at a purity of 99.5 mol% cumene with an impurity of 0.44 mol% benzene and 0.05 mol% DIPB. This stream exits at 236°C and 6 bar. The bottoms stream, DIISO, exits at 304°C and 6 bar with a purity of 98.6 mol% DIPB with an impurity of 1.4 mol% cumene. Both of these purities reach the requirements needed for the sale of the products.

The following table shows the mass balances for the plant, showing that the plant does conserve mass and the Aspen simulation is accurate.

Table 3: Mass flow streams entering and exiting the reactor and the major equipment, and the change across the equipment. Flow rates are in kg/hr.

Stream	Mass Flow	Stream	Mass Flow
Feed	12539.3	R-101 Inlet	12937.4
R-101 Feed	12937.4	R-101 Outlet	12937.4
R-101 Outlet	12937.4	R-101 Change	0
T-201 Feed	12937.4	T-201 Inlet	12937.4
T-201 Distillate	744.898	T-201 Outlet	12937.4
T-201 Bottoms	12192.5	T-201 Change	0
T-301 Feed	744.898	T-301 Inlet	744.898
T-301 Distillate	346.815	T-301 Outlet	744.898
T-301 Bottoms	398.083	T-301 Change	0
T-401 Feed	12192.5	T-401 Inlet	12192.5
T-401 Distillate	11736.6	T-401 Outlet	12192.5
T-401 Bottoms	455.954	T-401 Change	0
		Total In	12539.3
		Total Out	12539.3
		Total Change	0

Table 3 shows that the mass balances around the reactor and all three distillation towers are all net zero change, as is the plant itself. This shows that the Aspen simulation is converging to conserve mass. This proves that the Aspen simulation is accurate at describing the process.

Reactor Process Overview

The cumene production method used in this process invokes the reaction of propylene and benzene over a proprietary catalyst in vapor phase to produce cumene with selectivity towards cumene at lower temperatures. Thus, a single pass co-current shell and tube plug flow reactor would allow for appropriate cooling. In order to design a functioning plug flow reactor, a comprehensive design approach must take into account reaction kinetics, pressure drop, temperature variation, coolant fluid, and individual component properties. Both Polymath and Aspen were used to simulate and optimize the reactor. Optimization of the reactor took into account several factors, including operational temperature, tube types and numbers, inert catalyst, coolant inflow, and relative reactant flowrates. This reactor is made of 500 ¾” schedule 40 carbon steel tubes, a catalyst to inert ratio of 30-70. The coolant used was water. The inlet flow rate was selected to be 107 kmol/hr of benzene, and 103 kmol/hr of propylene with a 5% impurity of propane. As a result of the process simulation used in the Aspen software, the cumene production goal of 100,000 metric tons per year was met with a reactor output flowrate of 97.52 kmol/hr of cumene. Additionally, 2.83 kmol/hr of DIPB was also produced. The remaining benzene flowing out of the reactor is 6.85 kmol/hr, which is to be purified and recycled back into the reactor. The designed reactor also incorporates a minimal pressure drop of only 1.75% from 40 bar.

For a full report on the reactor design process, results, and evaluations, see Appendix A: Reactor Design.

Separation Process Overview

The goal of this design process is to produce cumene product at 100,000 metric tons per year with a purity of at least 99.5 mol%. Distillation was selected as the primary method to separate cumene from propane, DIPB, and benzene. Three distillation columns in series were employed to purify the cumene product. These columns were sized in order to maximize stream purity while minimizing size and cost. The first column, T-201, is fed the total mixture of the four components and separates benzene, propane, and propylene from the cumene and DIPB. In this column, benzene is treated as the heavy key and cumene as the light key. T-201 is a trayed column containing 19 sieve trays with a height of 15.24 m and a diameter of 0.76 m. The distillate from T-201 then enters T-301. T-301 separates propane and propylene from benzene. This is a low energy-intensive process so the column is small in comparison to the other two. Due to its small size, T-301 is a packed column consisting of 4 equilibrium phases with a height of 5.48 m and a diameter of 0.31 m. The bottoms containing benzene at 96.4% purity are then recycled back into the reactor. The bottoms of T-201, the stream containing cumene and DIPB, enters T-401. This column separates the cumene at 99.5% purity from the DIPB at 98.6% purity. Both of these purities meet or exceed the requirements for sale. T-401 is a trayed column containing 23 sieve trays with a height of 17.68 m and a diameter of 1.37 m. Other process designs were studied for this separation, most notably three columns with the bottoms of each feeding to the next column. Other methods of separation were explored, but were determined to be inappropriate for the necessary separation.

For a full report on the separation design process, results, and evaluations, see Appendix B: Separation Process Design.

Description of Equipment/Design Process

A check valve, VL-101, is used at the juncture of the recycle and the feed streams. The check valve is designed to not allow any backflow from the inlet or the recycle stream. The recycle stream has a small flow rate compared to the feed stream, and the prevention of backflow is needed to stop the possibility of the feed stream flowing backwards through the junction of the feed and recycle streams.

Heating and cooling process streams is an integral part of a chemical production process. Heat exchangers are used for transferring heat from one stream to another, and fired heaters are used to generate heat from a combustion reaction. The fundamental equation for heat exchangers is:

$$Q = UAF\Delta T_{ln}$$

Where Q is the heat transferred, or heat duty, U is the heat transfer coefficient, A is the heat transfer area, F is the correction coefficient, and ΔT_{ln} is the log mean temperature difference.

The largest heat exchanger in the plant is HE-101, which pre-heats the reactor feed while simultaneously cooling the reactor product stream. The heat exchanger was designed as a shell-and-tube model, with a heat transfer area of 22.77 m². The product stream from the reactor is the hot stream, and is cooled from 332°C to 180°C, and condensed from all vapor to all liquid. The cold stream is the reactor feed, which is preheated from 33°C to 210°C, and boiled to a vapor.

The heat exchanger is designed to run countercurrently, which allows for the outlet temperature of the hot stream to be lower than the outlet of the cold stream. The total heat duty of the exchanger is 2,196 kW. Figure 1 below shows the temperature profile for the heat exchanger.

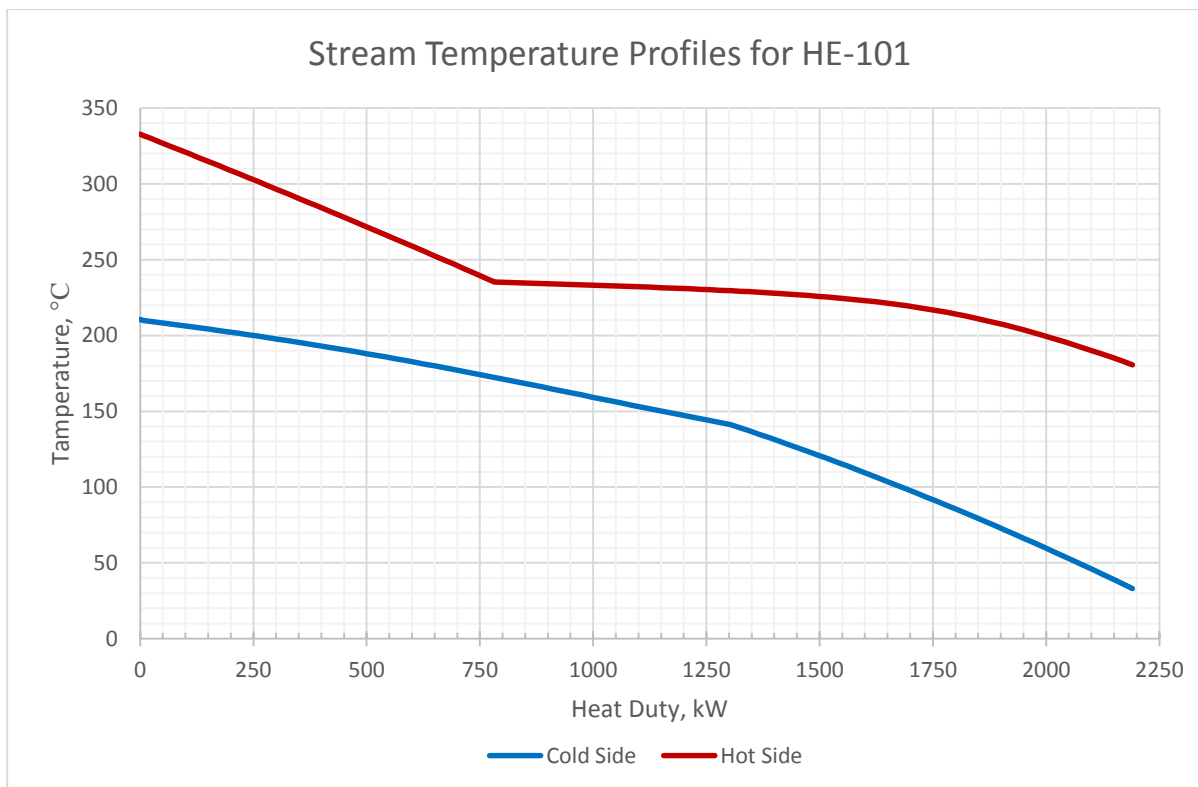


Figure 4: Stream Temperature Profile for Heat Exchanger 101, showing the Cold and Hot streams over the length of the exchanger, measured by heat duty.

Figure 1 shows that the hot side decreases to 235°C linearly, then becomes almost linear before sloping downward. This corresponds to the phase change starting at 235°C, then the liquid becoming subcooled as more vapor condenses. The cold side enters from the right side of the graph, and begins heating up to reach the final temperature of 210°C. The cold side stream is boiling over the majority of the exchanger, and the vapor is becoming superheated as the liquid fraction decreases.

Looking at the heuristics for heat exchangers, the heat transfer coefficient for a condenser is 850 W/m²°C. This value gives an F=0.85. This is an acceptable value for a condensing system. The shell for the heat exchanger has a 60 cm diameter, allowing for up to 37.2 m² of heat exchanging area, using 1" triangular spacing of ¾" OD piping, 16 ft long. The heat exchanger will have 777 tubes, and both the tubes and the shell are made of carbon steel as both streams are the hydrocarbons used in the reaction. The heat exchanger is used as a preheater, due to the log mean temperature difference being over 100° for cooling water. Using water would waste large amounts of thermal energy which can be recycled in the preheating process.

The reactor feed leaves the preheating exchanger HE-101 then proceeds into the fired heater, HE-102. The fired heater is sized for a maximum heat duty of 3624 kW, though only 1434 kW are needed during steady state operations. The fired heater was sized so that it could provide the full heating necessary to raise the feed to reactor specifications if the preheater was not operational. This is the case during the start-up of the plant, during the unsteady state operating conditions. The heater is made of carbon steel.

Two final heat exchangers complete the plant design, HE-301 and HE-401. Both heat exchangers are designed to cool the inlet streams into their respective distillation columns. HE-301 has a heat duty of 68.8 kW, and HE-401 has a heat duty of 320 kW. Both heat exchangers are water-cooled, and have a $U=850 \text{ W/m}^2\text{C}$. A correction factor of 0.9 is assumed from heuristics, as there is no phase change occurring, and gives a conservative estimate for area. Both heat exchangers are cooled with water, with an inlet temperature of 30°C and an outlet temperature of 45°C. The area for HE-301 is 1.4 m², and the area for HE-401 is 2.3 m². The design chosen for these two heat exchangers is double pipe, as it is a simple design, and is useful for small area applications. Even though the two heat exchangers cost under \$30,000 combined, they greatly improve the separations in the distillation columns they feed into.

There is one major pump in the process, P-101. The pump is a centrifugal pump with a required output of 39 kW, or 52.5 hp. The pump that was priced was 60 hp, so as to choose a standard sized pump available on the market. The higher horsepower also allows for a performance decrease over the lifespan of the pump that does not cause pressure problems in the process. The efficiency used was 0.50, as the pump was increasing the pressure from 1 bar to 40.5 bar. The reactor operates at 40 bar, and the expected pressure drop across the preheater and fired heater is 0.5 bar total. The pump was positioned before heating so that the pressure change occurred when the stream was a liquid, instead of a superheated gas.

A throttle valve, VL-102, is installed after the reactor to lower the pressure from 39.3 bar to 6.17 bar. The first distillation column was designed to operate at 6.0 bar, so the valve releases a slightly higher pressure to account for the pressure drop across the heat exchanger. The valve only interacts with a vapor stream, and only vapor is present after the valve. No liquid or solids should be present to cause any clogging in the valve.

Health and Environmental Considerations

Design of any chemical process involves health and environmental considerations, and the cumene production process is no exception. The safety of workers from chemical exposure is a prime factor in any plant design. The compounds involved in this process include benzene, cumene, DIPB, propylene, propane, and water as a coolant. Each of these compounds are exposed to high and low temperatures and pressures at different points in process. Benzene, cumene, and DIPB are all volatile liquids at room temperature and pressure, while propane and propylene are gases. All compounds are considered volatile organic compounds (VOCs) with several legal regulations to minimize output from chemical plants.

Propane, an impurity from the input of benzene in this chemical process, also acts as an inert in the reaction. The remaining propane entering the reaction is distilled off and used as a fuel gas to reduce waste and energy usage. Propane in itself is not toxic at low levels. However, at higher levels of exposure (>0.1%), propane can act as a central nervous system (CNS) depressant. Asphyxia is a possibility at high concentrations from reduced oxygen concentration. Since propane is a colorless and odorless gas, it is hard to detect if a leak occurs. Symptoms of propane toxicity are feelings of drowsiness and loss of consciousness. Propane is heavier than air and will flow lower to the ground when in gas form. Propane is a flammable gas at a lower flammability limit (LFL) of 2.1% in air and an upper flammability limit (UFL) of 10% in air. Use of propane as a fuel gas allows possibility of environmental leakage in gas. However, since it lacks reactive functional groups it is deemed as a safe compound for release in gas. The half-life of propane in the atmosphere is 14 days. Because propane is extremely volatile, even leakage into water will result in complete vaporization within a few hours (NLM Toxnet: Propane 2009).

Propylene is used primarily as a reactant in this process. It is in highest quantities before the reactor, but is not found in any stream downstream from the reactor. Propylene has similar physical properties to propane. The health effects of propylene are similar to the CNS depression found at high concentrations in propane, but are not as severe. Asphyxia is a possibility at high concentrations from reduced oxygen concentration. Propylene acts similar as a gas to propane in that it is odorless, colorless, and is heavier than air. The LFL and UFL of propylene are 2% and 11.1%, respectively. Propylene has a minimal environmental impact, is volatile in water leakage, and has a half-life in the atmosphere of 26 days (NLM Toxnet: Propylene 2014).

Benzene is another reactant found in the cumene production process. However, benzene is found in nearly every stream in this process since it is recycled. Benzene is heavier than propane and propylene, and tends to exist as a volatile liquid at room temperature. Benzene liquid is clear, but has a sweet odor and is slightly soluble in water. Benzene toxicity can have a wide range of health effects. Exposure to gas phase benzene in high concentrations has been shown to lead to acute CNS depression with abnormal cardiac rhythm that can lead to ventricular fibrillation or asphyxia. Ingestion of benzene can cause intestinal irritability including vomiting. Long term exposure to benzene can result in bone marrow damage leading to hematological problems such as leukemia and can act as an immunosuppressant. Benzene is also flammable with a LFL and UFL of 1.2% and 7.8%, respectively. In the atmosphere, benzene has been shown to form some ozone compounds (but at relatively low levels) and has a half-life of 17 days. Benzene can also result in toxicity to animals if leaked into soil or water, leading to reproductive problems (NLM Toxnet: Benzene).

Cumene is the primary product formed in this chemical process. The highest concentrations of cumene are found after the reactor and downstream in the separation processes. Cumene exists as a volatile liquid at room temperatures and pressures that is not soluble in water. As a gas, cumene can act as a CNS depressant much like benzene, and can do so at lower concentrations. There is some indication of abnormal cardiac rhythms with cumene exposure. The long term effects of cumene are largely unknown, but do not appear to be as toxic as benzene since cumene is readily metabolized in the body. Long term exposure in workers shows some evidence of

altered bilirubin and liver enzymes, indicating probable hepatic damage. Long term exposure also mimics bone marrow and hematological damage found in benzene. Cumene may also slightly irritate the eyes and skin. Cumene is a flammable liquid with a LFL and UFL of 0.9% and 6.5%, respectively. Atmospheric release of cumene has an approximate half-life of 1.5 hours and does not appear to significantly affect ozone levels. Cumene shows no indication of harm in environmental life at low concentrations and volatilizes in water (NLM Toxnet: Isopropylbenzene 2014).

P-Diisopropylbenzene (DIPB) is the only byproduct produced in this process. It is not produced in high quantities relative to cumene and is only found in high concentrations downstream in the separation process. DIPB, like cumene, exists as a volatile liquid at standard conditions and is not soluble in water. DIPB affects humans similarly to all other compounds in this process in that it acts as a CNS depressant at high levels. Lower level exposure can lead to burns on the skin and in the respiratory tract. Effects of long term exposure remain largely unknown, but has been shown to lead to bone marrow damage and subsequent hematological effects including leukemia and anemia. DIPB is a flammable liquid with a LFL and UFL of 0.8% and 6.5%, respectively. DIPB does not show any indication of harm towards environmental life. DIPB also volatilizes in water and is a VOC with a half-life of 30 days (NLM Toxnet: Diisopropylbenzene 2003).

This process attempts also attempts to minimize environmental impacts as the result of carbon emissions from energy usage, and from waste prevention. The separation flow process, for instance, was designed in a specific order to significantly reduce the size and utility requirements for one of the columns. The design of a heat exchanger that uses two existing streams (reactor outflow and feed stream) in the process to exchange energy between the two also lowers required energy consumption into the process. This internal conservation of energy within the process not only lowers utility costs for the plant, it reduces the potential environmental impact of the chemical production industry as a whole. Additionally, all products formed from this process are either sold or recycled. The cumene and DIPB products are moved into the petrochemical plant for further processing. The benzene stream is recycled back into the reactor to save costs from new benzene input. Finally, the propane distilled off from the process is used as a fuel gas, further reducing utility requirements of the plant. Overall, this process produces no chemical waste, and makes a great use of internal energy to reduce environmental impact into the 21st century and beyond.

Process Controllability, Instrumentation, and What-If Hazard Analysis

Assuming this project is approved, greater design detail will be required for full process integration. This future design will include all necessary controls, piping, and instrumentation to operate a complete process from startup to shut down. An example of a future piping and instrumentation diagram for one piece of equipment is shown in Figure 5. This P&ID includes distillation tower T-201, the equipment necessary for its operation, and the various valves and safety controls around these pieces of equipment.

During the formulation of this P&ID, process safety and controllability is kept in mind. As shown, there are many temperature, flow, and pressure indicators. These allow for operators to monitor the process. Some of these are in control loops to prevent spills, leaks, or other potentially hazardous conditions. There are three places on the column where temperature and pressure are monitored. These include right at the feed stream, in the top, and towards the bottom. This gives the operators a good view of the process, so they are able to observe if an upset has occurred.

Through the distillate, there is another temperature indicator past the condenser. Past the condenser is a small vessel that can hold distillate to allow the pump to maintain a steady flow to reflux, as well as to the next stage of the process. This vessel has a level indicator, along with low and high alarms which will alert operators to a potential problem. There are two reflux pumps, which are automatically set to run one at a time. This way if one pump goes down or needs repairs, the other can run the process. Past the pump, a flowmeter is connected to a control valve to maintain a steady reflux rate.

The bottoms flow also has control loops to maintain a steady flow. The first is a flowmeter that connects to a control valve to either close, which forces more liquid through the reboiler or open to allow the stream to continue through the process. Once through the reboiler, there is a temperature indicator which controls the flow of steam to maintain a steady temperature.

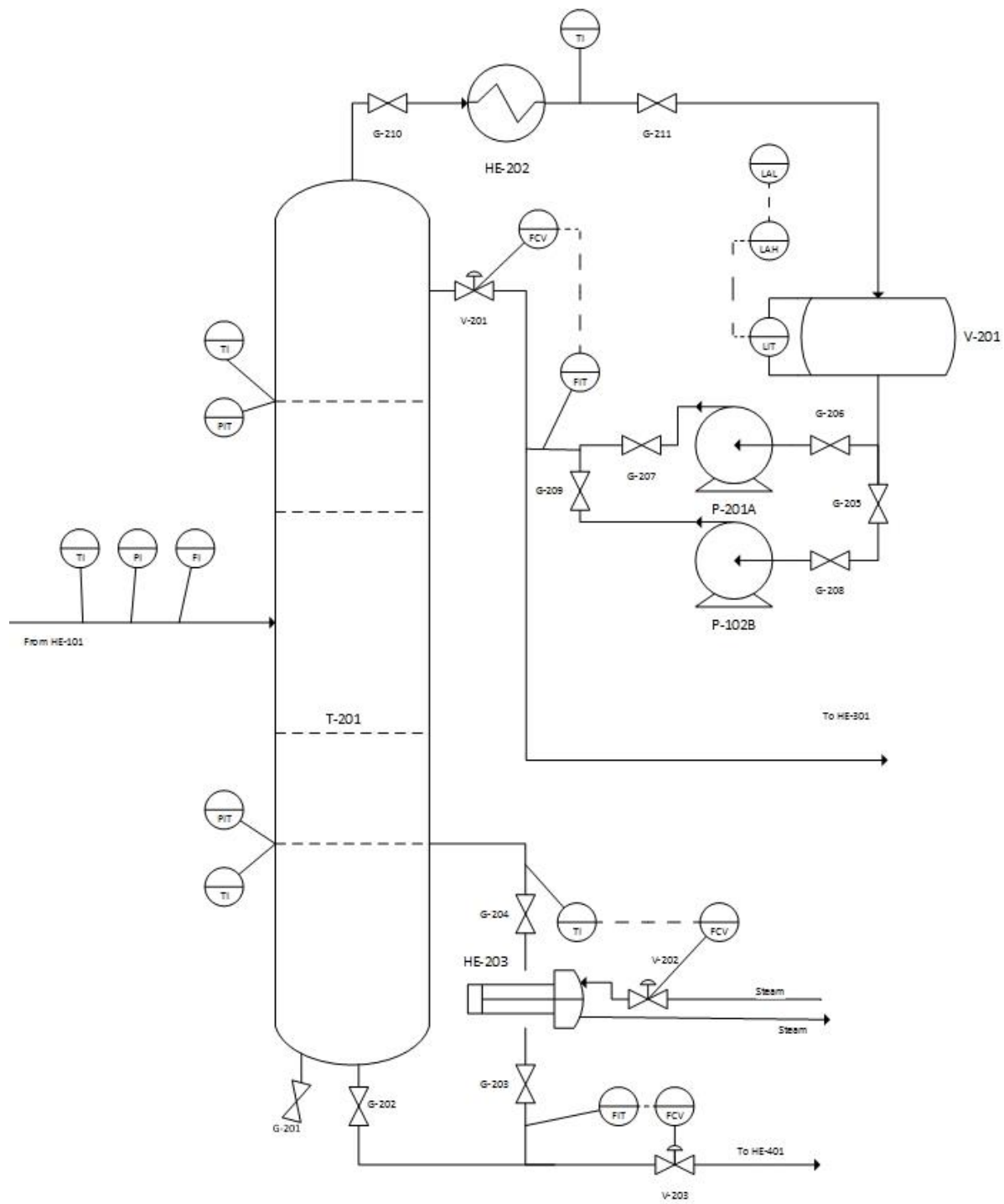


Figure 5. Preliminary piping and instrumentation diagram around T-201 distillation column

Another consideration is safety and hazard analysis. While many of the concerns in the What-If analysis are accounted for in the design, care is still be taken to ensure the process runs safely and smoothly. The following is a summary of the analysis completed using the P&ID provided above.

- What if the feed temperature is higher or lower than specified?
 - Personal protection equipment (PPE) includes gloves and full arm and leg covering. This will protect from potential burns from the outside of the pipe. Additionally, this should not pose a safety threat, only create a worse separation.
- What if the flow from the top to the condenser is more or less than specified?
 - The vessel after the condenser will keep any excess liquid produced during high flow, or allow for that excess liquid to be used during low flow. A level alarm is included to prevent overfilling. This poses no safety risk.
- What if the reflux pump goes down?
 - The control panel automatically will switch the other pump on, preventing a pressure buildup. Pumps can also be manually turned on from the control room to allow for pump repairs.
- What if the flow from the bottoms is higher or lower than specified?
 - A flowmeter is connected to a control valve to prevent too much or too little going through the reboiler. This will mitigate pressure issues.
- What if the reboiler is heating the stream too much or too little?
 - A temperature indicator is connected to a flow control valve on the hot side of the reboiler.
- What if the sample port leaks while taking a sample?
 - PPE is required in the plant at all times, and includes safety glasses. Additional PPE for taking a sample includes a full face mask.

Economic Evaluation

The most important aspect of plant process design is the economics behind the plant's construction and the future value. The initial year for the plant is 2013, and all prices and discounts will reference to 2013 dollars. All equations used in economic analysis are included in appendix C. The economics will be displayed in four categories: fixed capital investment, capital costs, depreciation, and discounted cash flow.

Fixed Capital Investment

The Fixed Capital Investment (FCI_L) for the project is expected to be \$25 million. This was calculated by multiplying the sum of the Total Module Cost (C_{TM}) and half the Bare Module Cost (C_{BM}) by the Lang Factor of a fluid processing plant, $F_{Lang}=4.74$. The Bare Module Cost is calculated in Table 4 below, which shows the equipment in the plant, the purchase cost, and C_{BM} . CapCost was used to price equipment, using the CEPCI for 2013, which is 567.3.

Table 4: Table of the purchase and bare module cost for all major equipment. Cost is in \$thousand.

Equipment Type	Equipment Name	Purchase Cost	C_{BM}
Reactor	R-101	42.9	145.0
Reboiler	HE-202	25.0	82.4
Reboiler	HE-302	22.0	72.7
Reboiler	HE-402	34.3	113.0
Pre-Heater	HE-101	23.4	83.7
Fired Heater	HE-102	826.0	1,830.0
Cooler	HE-301	3.5	11.4
Cooler	HE-401	4.0	12.9
Compressor	P-101 A/B	22.5	124.0
Reflux	P-102 A/B	7.0	27.9
Reflux	P-103 A/B	7.0	27.9
Reflux	P-104 A/B	7.0	27.9
Condenser	HE-203	31.6	68.5
Condenser	HE-303	29.7	64.4
Condenser	HE-403	43.9	95.4
Column	T-201	33.8	75.1
Column	T-301	3.4	13.3
Column	T-401	71.6	198.0
Cond Accum	V-201	6.5	21.2
Cond Accum	V-301	6.5	21.2
Cond Accum	V-401	8.0	27.3
Total		1,259.5	3,143.2

The total C_{BM} is just under \$3.15 million. This yields a C_{TM} of \$3.7 million. This gives a FCI of \$25 million. Working capital is 17.5% of the FCI_L , giving a working capital of \$4.4 million.

Capital Costs

The Direct Capital Costs (C_D) is \$127.6 million/year, with raw materials consisting of over 95% of the total. The full breakdown of the Direct Capital Costs is shown in Table 5. Further breakdowns of raw materials and utilities are in Tables 6 and 7 below. The prices for materials are from ICIS and utility prices from Wildcat Petrochemical's preliminary research are assumed to be 2013 values.

Table 5: Table of the cost factors for the capital costs. Cost is in \$thousand

Cost Factor	Cost (\$thousand)
Cost of Labor	953
Supervisory and Clerical	167
Maintenance and Repairs	1,502
Operating Supplies	225
Laboratory Charges	143
Raw Materials	122,472
Utilities	2,189
Proprietary Catalyst	1.04
Plant overhead	1,576
Administrative	394
Total	129,621

Table 5 includes the prices of all streams entering or leaving the process. The first two are reactant streams containing benzene and propylene. These streams are included in the material cost, which accounts for the majority of direct capital costs. The next two rows are the product streams, which are revenue producing.

Table 6. Annual material costs and prices of reactants and products. Propylene/propane and benzene are costs, and cumene and DIPB are profits.

Material	Price (\$/kg)	Flowrate (kg/h)	Annual price
Propylene/Propane	1.12	4557.26	\$45,552,468
Benzene	1.20	7982.84	\$79,919,133
Cumene	1.37	11736.6	\$133,419,932
DIPB	3.30	455.96	\$12,521,737

Table 6 shows the utility costs for various pieces of equipment. HE-101 is not included since it does not use outside utilities. HE-102 uses natural gas, but we account for a fuel gas credit from our propane distillate from T-301. The reboilers all use low-pressure steam while the pumps require electricity. Cooler HE-201 uses cooling water, while HE-301 needs refrigerated water. All utility prices are from Wildcat Petrochemicals, Inc. and are assumed to be 2013 values.

Table 7. Yearly utility costs.

Equipment	Energy	Utility cost	Yearly cost
HE-102	42120 GJ	11 \$/GJ	\$370,647
HE-202	7465 GJ	13.28 \$/GJ	\$99,113
HE-203	22880 GJ	13.28 \$/GJ	\$303,827
HE-301	2030 GJ	0.354 \$/GJ	\$719
HE-302	1825 GJ	13.28 \$/GJ	\$24,215
HE-303	2660 GJ	13.28 \$/GJ	\$35,312
HE-401	9430 GJ	\$4.43 \$/GJ	\$41,763
HE-402	29690 GJ	13.28 \$/GJ	\$394,299
HE-403	64215 GJ	13.28 \$/GJ	\$852,778
P-101	320554 kWh	0.06 \$/kWh	\$19,233
P-201	82000 kWh	0.06 \$/kWh	\$4,920
P-301	82000 kWh	0.06 \$/kWh	\$4,920
P-401	82000 kWh	0.06 \$/kWh	\$4,920
R-101	90200 GJ	0.354 \$/GJ	\$31,931

Depreciation

The depreciation method used is the modified accelerated cost recovery system, or MACRS. This utilizes a hybrid of the double declining and the straight line methods. In addition, a half-year convention is employed. The depreciation values are shown below in table 8.

Table 8. Yearly depreciation values using 6 year schedule MACRS with a half year convention.

Year	MACRS	SLD
1	\$ 5,005,986	
2	\$ 8,009,578	\$ 4,449,765
3	\$ 4,805,747	\$ 3,432,676
4	\$ 2,883,448	\$ 2,883,448
5		\$ 2,883,448
6		\$ 1,441,724

Discounted Cash Flow

While completing economic analysis, all future value money was discounted to year 2013 using the minimum acceptable rate of return as 15% p.a. Figure 6 below shows the discounted cash flow diagram. It is apparent that this project is favorable, since the net present value is significantly above the break-even point. The discounted payback period is four years after the start of production, or six years after the start of the project. Since the life of the plant will be

more than 15 years, the income provided from this plant will continue to grow past the scope of this analysis.

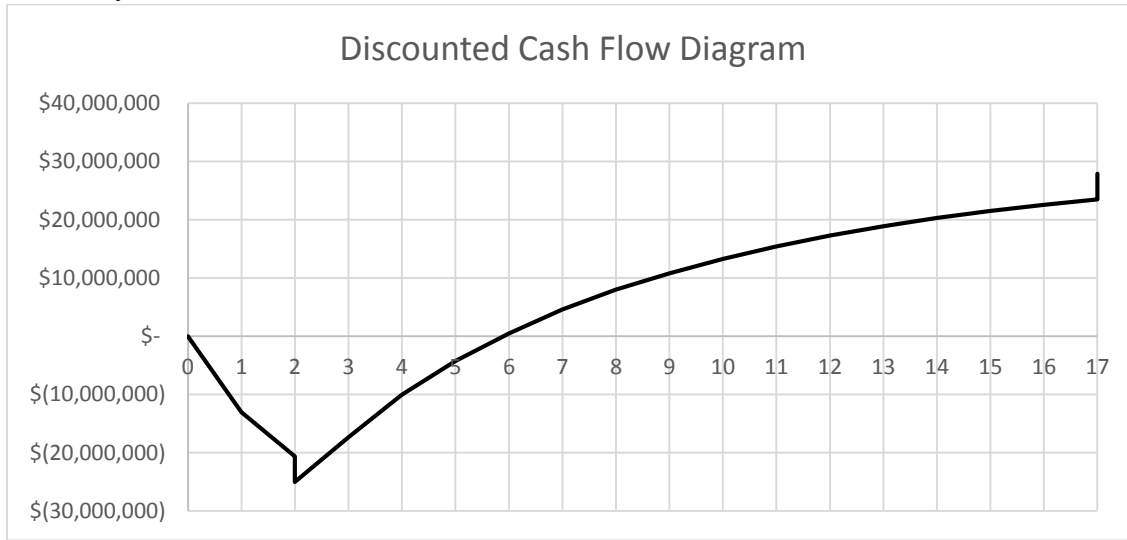


Figure 6. Cash flow diagram discounted to 2013 starting with year 0 as the start of construction of the plant, and production starting at year 3.

Table 9 shows a yearly breakdown of the data used to create the diagram in Figure 6.

Table 9. Yearly taxes, discounted net cash flow, and cumulative discounted cash flow. Year 2 includes working capital as an expense in the cumulative column while year 17 includes working capital as a profit returned.

Year	Taxes	Discounted net cash flow	Cumulative discounted cash flow
1	\$ -	\$ (13,059,000)	\$ (13,059,100)
2	\$ -	\$ (7,570,000)	\$ (20,629,600)
3	\$ 4,649,000	\$ 7,674,000	\$ (17,336,100)
4	\$ 3,598,000	\$ 7,274,000	\$ (10,062,200)
5	\$ 4,720,000	\$ 5,768,000	\$ (4,294,600)
6	\$ 5,392,000	\$ 4,724,000	\$ 429,800
7	\$ 5,392,000	\$ 4,108,000	\$ 4,538,000
8	\$ 5,897,000	\$ 3,407,000	\$ 7,945,400
9	\$ 6,402,000	\$ 2,820,000	\$ 10,764,900
10	\$ 6,402,000	\$ 2,452,000	\$ 13,216,600
11	\$ 6,402,000	\$ 2,132,000	\$ 15,348,600
12	\$ 6,402,000	\$ 1,854,000	\$ 17,202,500
13	\$ 6,402,000	\$ 1,612,000	\$ 18,814,600
14	\$ 6,402,000	\$ 1,402,000	\$ 20,216,400
15	\$ 6,402,000	\$ 1,219,000	\$ 21,435,400
16	\$ 6,402,000	\$ 1,060,000	\$ 22,495,400
17	\$ 6,402,000	\$ 922,000	\$ 27,797,338

Conclusions and Recommendations

The process design presented for cumene production uses benzene and propylene to produce cumene using a proprietary catalyst. The process design includes three distillation columns for purifying the products and the recycle. Considerations were taken on column order and sizing, and on conversion of thermal energy throughout the process. The plant design will generate 97.8 kmol of cumene per hour, with an annual production of 96.2 thousand tonnes.

The design has a capital investment of \$25 million over the two years of construction. Using a 5 year MACRS depreciation model, the project has a discounted payback period of 4.0 years after start-up. The net present value of the project is \$27.8 million, with a minimal accepted return rate of 15%.

From the final design and the calculated economic review, the recommendation is to begin final design and start construction as soon as possible. The plant has a high annual output, and has a large profit potential. The health hazards of the components are that of any organic compound processing facility, and the safety technology can be implemented to minimize the potential for any dangerous incidents. The process will have a short payback period, so investors will be interested in the project if the company does not have the required capital to initially invest.

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Appendix A: Reactor Design

Submitted to:
Dr. Keith Hohn
CHE 550

Submitted by:
Tristan Grieves, Nikki Klaassen, Patrick O'Connor, Sarah Keffer

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Appendix A: Reactor Design

A.1 Executive Summary

The cumene production method used in this process invokes the reaction of propylene and benzene over a proprietary catalyst in vapor phase to produce cumene. As a byproduct, p-diisopropylbenzene (DIPB) is also produced. The method of this reaction makes it appropriate for the use of a co-current shell-and-tube plug flow reactor. Optimization of the reactor took into account several factors, including operational temperature, tube types and numbers, inert catalyst, coolant inflow, and relative reactant flowrates. This reactor is made of 500 ¾” schedule 40 carbon steel tubes, a catalyst to inert ratio of 30-70. The coolant used was water. The inlet flow rate was selected to be 107 kmol/hr of benzene, and 103 kmol/hr of propylene with a 5% impurity of propane. As a result of the process simulation used in the Aspen software, the cumene production goal of 100,000 metric tons per year was met with a reactor output flowrate of 97.52 kmol/hr of cumene. Additionally, 2.83 kmol/hr of DIPB was also produced. The remaining benzene flowing out of the reactor is 6.85 kmol/hr, which is to be purified and recycled back into the reactor. The reactor side of the process minimalizes the hotspot with a maximum temperature change of only 10.1 °C. The designed reactor also incorporates a minimal pressure drop of only 1.75% from 40 bar.

A.2 Introduction

The production of cumene involves multiple reactants in vapor form and catalyst particles; thus the reaction is perfectly suited for a plug flow reactor. Cumene formation is an exothermic reaction, with selectivity towards cumene at lower temperatures. This indicates it is probably necessary to cool the reaction while it is taking place to prevent reaction runaway or selectivity toward a byproduct, p-diisopropylbenzene (DIPB). Thus, a single pass co-current shell and tube plug flow reactor would allow for appropriate cooling. In order to design a functioning plug flow reactor, a comprehensive design approach must take into account reaction kinetics, pressure drop, temperature variation, coolant fluid, and individual component properties. Both Polymath and Aspen were used to simulate and optimize the reactor.

A.3 Equations

To begin the process of designing the reactor, the necessary equations to be solved are listed below. There are three basic sets of equations to be solved: mole balances for all species, the energy balance for both co-current and counter-current flow, and the momentum balance.

A.3.1 Variables

$G \equiv$ superficial mass velocity

$\Phi \equiv$ bed porosity

$D_p \equiv$ particle diameter

$D \equiv$ diameter of tube

$N \equiv$ number of tubes

μ \equiv viscosity
 ρ \equiv catalyst density
 U \equiv overall heat transfer coefficient
 a \equiv heat transfer area
 A \equiv cross sectional area
 P \equiv pressure
 C_i \equiv concentration of component i
 F_i \equiv flow rate of component i
 C_{p_i} \equiv heat capacity of component i
 \dot{m}_c \equiv flow rate of coolant
 $C_{p_{cool}}$ \equiv heat capacity of coolant
 z \equiv position in reactor

A.3.2. Mole Balances

Propylene:

$$\frac{dF_A}{dz} = A\rho(-k_1 C_A C_B - k_2 C_A C_C)$$

Benzene:

$$\frac{dF_B}{dz} = -A\rho k_1 C_A C_B$$

Cumene:

$$\frac{dF_C}{dz} = A\rho(k_1 C_A C_B - k_2 C_A C_C)$$

DIPB:

$$\frac{dF_D}{dz} = A\rho k_2 C_A C_C$$

Propylene:

$$C_A = C_{T_0} \frac{F_A T_0 P}{F_T T P_0}$$

Benzene:

$$C_B = C_{T_0} \frac{F_B T_0 P}{F_T T P_0}$$

Cumene:

$$C_C = C_{T_0} \frac{F_C T_0 P}{F_T T P_0}$$

DIPB:

$$C_D = C_{T_0} \frac{F_D T_0 P}{F_T T P_0}$$

Propane:

$$C_I = C_{T_0} \frac{F_I T_0 P}{F_T T P_0}$$

A.3.3 Energy Balances

Co-Current Flow Coolant:

$$\frac{dT_a}{dz} = \frac{Ua\pi R^2 [T(z) - T_a]}{\dot{m}_c * C_{p_{cool}}}$$

Counter-Current Flow Coolant:

$$\frac{dT_a}{dz} = \frac{Ua\pi R^2 [T_a - T(z)]}{\dot{m}_c * C_{p_{cool}}}$$

Heat of Reaction:

$$\Delta H_{Rx}(T) = \Delta H_{Rx}^\circ(T_R) + \int_{T_R}^T \Delta C_p dT$$

Reactor Temperature:

$$\frac{dT}{dz} = \frac{A * Ua(T_a - T) + A * \rho \sum_{i=1}^n [(-\Delta H_{iRx}(T) * r'_{ij})]}{\sum_{i=1}^m F_i C_{p_i}}$$

A.3.4 Momentum Balance Derived From Ergun Equation

$$\frac{\partial P}{\partial z} = \frac{G}{\rho * g_c * D_p} \left(\frac{1 - \phi}{\phi^3} \right) \left[\frac{150(1 - \phi * \mu)}{D_p} + 1.75 * G \right] \left(\frac{P_0}{P} \right) \left(\frac{T}{T_0} \right) \left(\frac{F_T}{F_{T_0}} \right)$$

$$G = \frac{\sum(F_{i0} * M_i)}{A_c}$$

$${}^1C_{p_A} = 0.1043 * T + 48.3$$

$${}^1C_{p_B} = 0.019 * T + 169$$

$${}^1C_{p_C} = 0.315 * T + 102.5$$

$${}^1C_{p_D} = 0.196 * T + 248.8$$

$${}^1C_{p_I} = 0.125 * T + 58.16$$

$${}^1\Delta H_{Rx1}^\circ(T_R) = -103892 \frac{J}{mol}$$

$${}^1\Delta H_{Rx2}^\circ(T_R) = -98550 \frac{J}{mol}$$

$$a = \frac{4}{D}$$

$$A = \pi \frac{D^2}{4}$$

$$F_T = F_a + F_b + F_c + F_d + F_i$$

$${}^2\rho = 1600000 \text{ g m}^{-3}$$

$$P_0 = 40 \text{ bar}$$

$$T_0 = 250.2 \text{ K}$$

$${}^2U = 60 \text{ W m}^{-2} \text{ }^\circ\text{C}^{-1}$$

$${}^1C_{p_{\text{cool}}} = 4.2 \text{ J/g}\cdot\text{K}$$

$$F_I = 0.1168 \text{ mol s}^{-1}$$

$$m_c = 2922.47 \text{ g s}^{-1}$$

$${}^2D_p = 0.003 \text{ m}$$

$${}^1\mu = 0.0000000204554 \cdot T + .000004784$$

$${}^1M_{\text{propylene}} = 42.08 \text{ g mol}^{-1}$$

$${}^1M_{\text{benzene}} = 78.11 \text{ g mol}^{-1}$$

$${}^1M_{\text{propane}} = 44.1 \text{ g mol}^{-1}$$

¹(Aspen Plus Version 8.8)

²Data provided from problem statement

A.4 Results

The reactor design reflects both the constraints provided by the task request as well as some considerations for future reports when optimizing overall plant costs. For basic design parameters of the single pass shell and tube plug flow reactor referred to in Table 1, the tubes were chosen to be produced out of common $\frac{3}{4}$ Schedule 40 stainless steel, with a total of 500 tubes. The inert packing, which allows for better control of reaction kinetics, was to be 70% of the reactor packing. Finally, the length of the reactor was 5.4 meters. The inlet temperature and initial flow rates were also selected based upon the suggested design parameters as shown in Table 2. An inlet temperature of 377.2 °C was used at a pressure of 40 bar. A flowrate of 107 kmol/hr of benzene and 103 kmol/hr of propylene, with an impurity of 5.03 kmol/hr of inert propane. With the inclusion of a recycle stream in the final process, the actual flow rates were 107.02 kmol/hr of benzene, 0.18 kmol/hr of cumene, 103 kmol/hr of propylene, and 5.03 kmol/hr of propane.

As a result, the reactor output of the primary product, cumene, was 97.52 kmol/hr. The output of the secondary product, DIPB, was 2.83 kmol/hr. Some of the reactants also exited the reactor, with 6.85 kmol/hr of benzene which can be separated off and recycled later in the process. The temperature of the reactor components stayed well within the recommended 20 °C, with a maximum temperature change from inlet temperature of only 10.1 °C. The exiting temperature was 372 °C, a decrease of 5.2 °C from inlet temperature. Finally, the pressure dropped 0.7 bar from the initial pressure of 40 bar (Table 2).

The coolant stream variables were selected in order to optimize the reaction, shown in Table 2. The flow rate of 584 kmol/hr of water was selected to be nearly the same as the flow of reactants on the reactor side. Water entered at 20 °C and 1 bar as a pure liquid and underwent a phase change to exit at 102.1 °C and 1 bar at 27.5% quality.

Table 10. Basic reactor design parameters used in Aspen. The inert packing percentage is directly proportional to reaction kinetics.

Number of tubes	500
Length (m)	5.4
Diameter (m)	0.02134
Inert packing	70%

Table 11. Stream table of cumene reaction process simulation as provided by Aspen. The resulting output of cumene is high enough to meet the goal of 100,000 metric tons per year.

		Coolant In	Coolant Out	Feed	Product
Cumene	kmol/hr	0	0	0	97.52
Benzene	kmol/hr	0	0	107.02	6.85
Propylene	kmol/hr	0	0	103	0
DIPB	kmol/hr	0	0	0	2.83
Propane	kmol/hr	0	0	5.03	5.03
Water	kmol/hr	584	584	0	0
Total Mole Flow	kmol/hr	584	584	215.23	112.23
Temperature	°C	20	102.1	360	376.601
Maximum Temp Difference	°C		80.1		10.1
Pressure	Bar	1	1	40	39.3
Quality		0	0.275	1	1

For the mathematical simulation performed in Polymath, the same input constants and temperatures were used as were used in Aspen. The resulting reaction did not proceed as far and the output stream contained 88.05 kmol/hr of cumene and 7.47 kmol/hr of DIPB. Reactants were much more abundant in the output stream, with 6.69 kmol/hr of benzene and 0 kmol/hr of propylene. The products exited at 399.4 °C and 39.75 bar. The coolant stream had a much larger temperature increase, up to an exit temperature of 326.4 °C (Table 3).

Table 3. Stream table of cumene reaction process simulation as provided by the mathematical model used in Polymath. When compared to the Aspen simulation, the reaction shows greater selectivity towards DIPB.

		Coolant In	Coolant Out	Feed	Product
Cumene	kmol/hr	0	0	0	88.05
Benzene	kmol/hr	0	0	107.02	6.69
Propylene	kmol/hr	0	0	103	0
DIPB	kmol/hr	0	0	0	7.47
Propane	kmol/hr	0	0	5.03	5.03

Water	kmol/hr	584	584	0	0
Total Mole Flow	kmol/hr	584	584	215.05	107.24
Temperature	°C	20	326.4	377.2	399.4
Maximum Temp Difference	°C		306.4		32.83
Pressure	Bar			40	39.73

A.5 Comparison of Aspen to Mathematical Model

The reactor design for cumene production was first mathematically modeled using Polymath. This mathematical model solved a series of governing differential equations as provided above in Section A.1 for species concentration, species flow rates, pressure change, temperature change of the reactant stream, and temperature change of the coolant over the length of the reactor. The design parameters determined in Polymath were then used to begin a simulation of the reactor in Aspen.

The concentration of each species follows different trends in both the mathematical model (Figure 2) and the Aspen simulation (Figure 1), and the reaction does not show quite as much selectivity towards cumene as it does in Aspen. The differing profiles are most likely directly related to the difference in temperature profiles between the two models (Figures 3 and 4). The difference in final concentration could be due to the models developed from provided data for heat of reaction and heat capacity of each species used when solving the differential equations in Polymath. The heat of reaction and change in heat capacity used in Aspen is a much more dynamic model that takes into account factors such as pressure and temperature change, and effects of mixing. In addition, Aspen uses a model for mass transfer through catalyst effects throughout the reactor, which was not used in the mathematical solution.

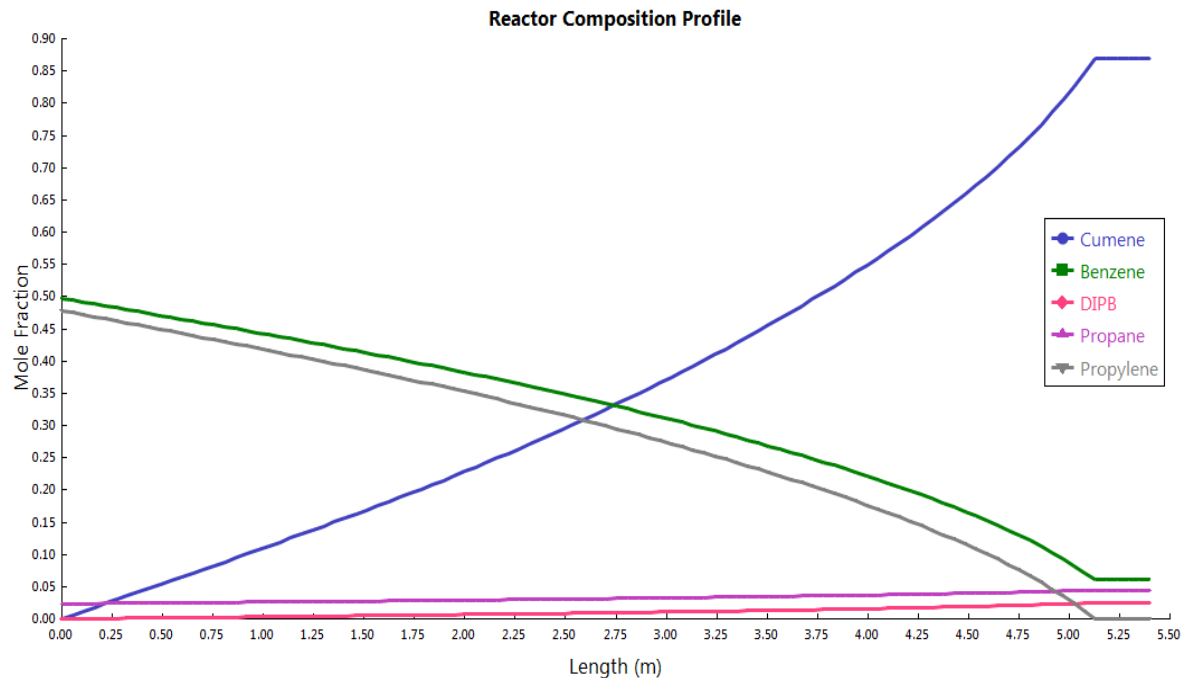


Figure 7. Molar composition of each component in reactor as a function of position of the Aspen simulation. The concentration near the end of reactor stops changing, which is due to the reaction being completed.

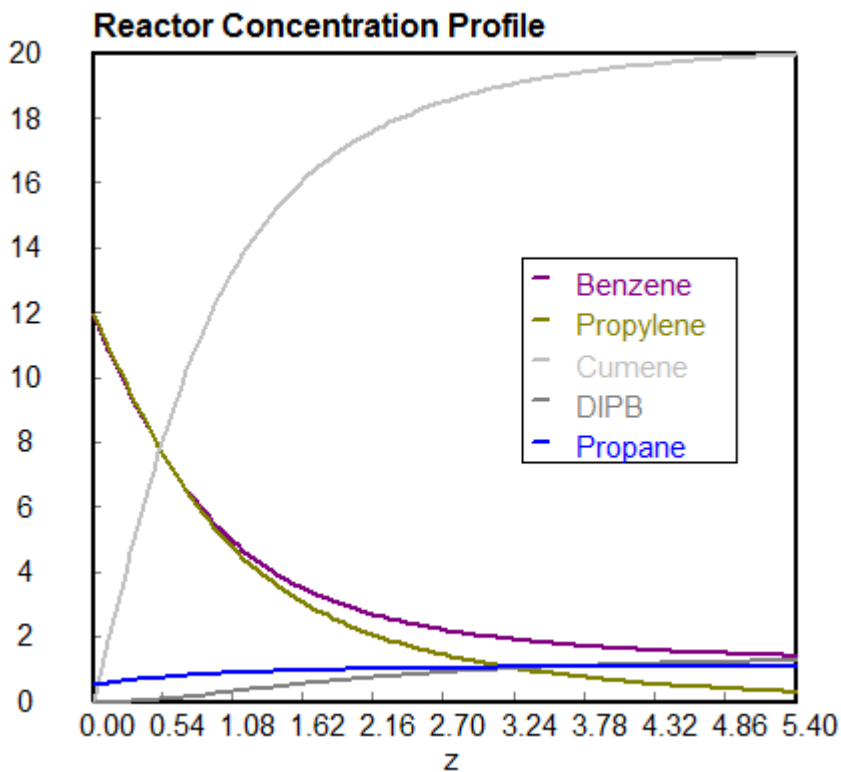


Figure 2. Polymath component concentration profile in reactor as a function of position. Notice the different curve profile found in the mathematical model as opposed to the Aspen model. The x-axis is in meters, while the y-axis represents relative compositions.

The co-current model was used in both the mathematical model and in Aspen. In the simulation completed in Aspen, the resultant coolant output stream reveals a phase change took place in the shell side of the plug flow reactor. In Polymath, this phase change was not modeled. The temperature profile for the mathematical model of the reactor (Figure 4) follows a similar trend in the Aspen simulation (Figure 3). The exit temperatures of both the mathematical simulation and Aspen are fairly similar. However, the coolant temperature continues to increase in the Polymath model but does not do so in the Aspen model. This is a direct result of the phase change, which was not taken into account over the length of the reactor. The model used in Aspen does take into account this steady phase change and the change in pressure resulting in a temperature increase (Figure 3).

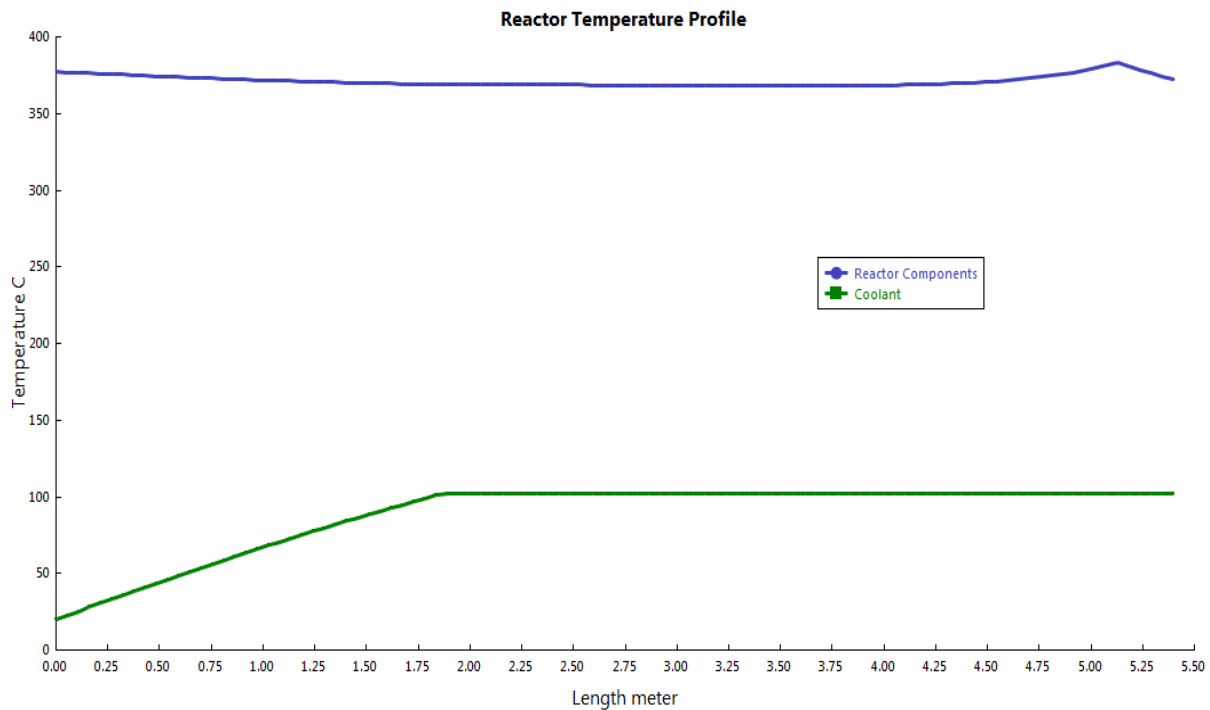


Figure 3. Temperature profile in reactor as a function of position of the Aspen simulation. The sudden temperature plateau of the coolant is due to a phase change taking place. The sudden spike in reactor component temperature near the end of the reactor is when the reaction is complete.

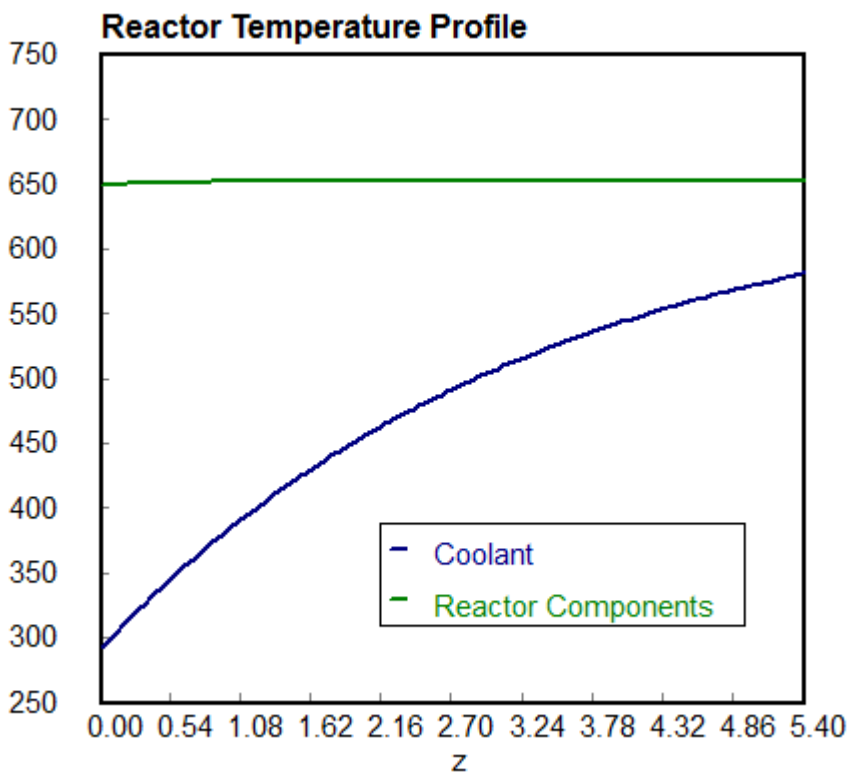


Figure 4. Polymath reactor and coolant temperature profile in reactor as a function of position. The temperature is in units of Kelvin on the y-axis. The x-axis is in meters. Notice the fairly flat temperature profile of the reactor components. Additionally, the coolant does not plateau. The Polymath model did not take into account phase change.

Both the Aspen simulation and the mathematical model use the same equation (Ergun equation) to approximate pressure drop. Thus, the final drop should be the same assuming the input and output temperatures and flow rates are approximately the same. However, the output flow rate of the Polymath model was slightly smaller than the output flow rate from the Aspen simulation. The resulting pressure drop in the mathematical model should therefore be smaller than the drop from the Aspen simulation. This holds true, as the change in pressure over the reactor in the Aspen simulation is 0.7 bar (Figure 5). The mathematical model yields a pressure drop of only 0.27 bar (Figure 6).

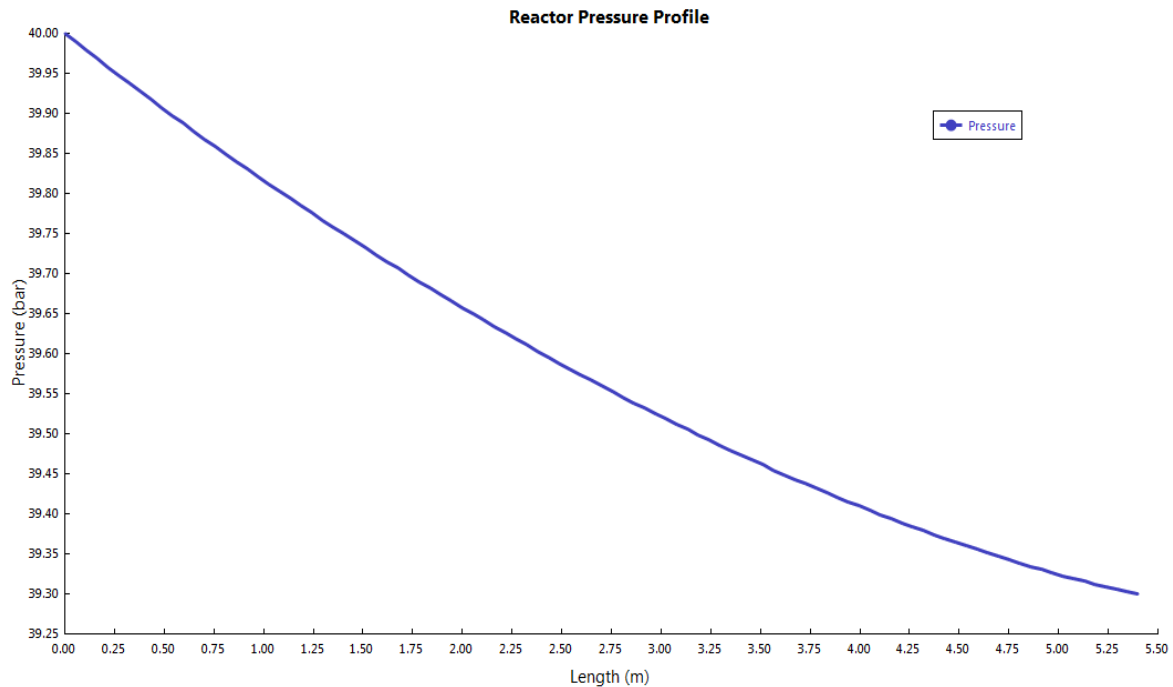


Figure 5. Pressure profile in reactor as a function of position of the Aspen simulation. The temperature profile decreases steadily.

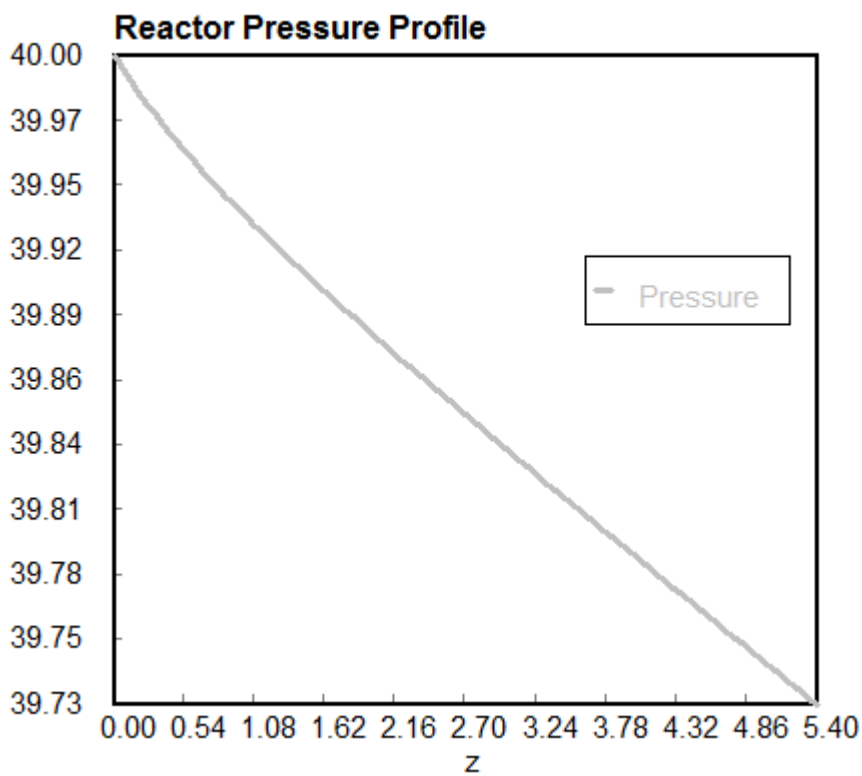


Figure 6. Polymath pressure profile in reactor as a function of position. The x-axis is in meters and the y-axis is pressure, in bar.

A.6 Design Discussion

Fully functional reactors depend on a number of different complex variables in order to balance production, cost, and safety. Some variables have less room for change than others. These include pipe diameter and the output flow rate. Pipe diameter is generally a standardized value based on what is available. The pipe diameter should be small but still several times the catalyst particle diameter. For this reactor, ¾ schedule 40 carbon steel piping was used. Carbon steel was used because it is cheap and the chemicals used have no considerable corrosive properties.

Flow rates are based on the desired output of cumene, and the output flow rate of 97.52 kmol/hr is adequate for the requested production of 100,000 metric tons per year. A flow rate of 107 kmol/hr of benzene and 103 kmol/hr of propylene, with an impurity of 5.03 kmol/hr of inert propane. With the inclusion of a recycle stream in the final process, the actual flow rates were 107.02 kmol/hr of benzene, 0.18 kmol/hr of cumene, 103 kmol/hr of propylene, and 5.03 kmol/hr of propane. This flow rate was selected to maximize production of cumene. While the selectivity towards cumene could theoretically be improved by dramatically increasing the inlet concentration of benzene, the cost of separating and recycling the benzene proves to be too high to make a difference in cost efficiency.

In order to fully optimize the reactor, the balance of several different parameters has to be taken into consideration. These include reactor length, inlet flow temperature, coolant temperature, percentage of inert catalyst, and number of tubes. The reactor length was chosen to allow appropriate length for the reaction to be completed (complete consumption of propylene reactant). The inlet flow temperature was chosen in order to balance reaction selectivity toward cumene while also maintaining an appropriate reactor length. The coolant inlet temperature allowed for a small temperature range (<20 °C change from inlet temperature) in the reactor and maintained an adequate reaction temperature. Much like the inlet temperature, the percentage of inert catalyst in the reactor can greatly affect reaction kinetics. A catalyst to inert ratio of 30 to 70 maximized reactor productivity while minimizing the reactor hot spot. As a result the temperature only varies 10.1 °C at most from the inlet temperature, preventing a runaway reaction. The number of tubes within the reactor plays a major role in the pressure drop across the reactor and tubular flow rate. The resulting pressure drop is only around 1.75% of the initial pressure, allowing the reaction kinetics to maintain a more constant value over the length of the reactor.

For this reactor, water was chosen as the coolant of choice for the reactor. The boiling point of water, at the pressure used is 100 °C. This means that the water in the cooling side of the reactor undergoes a partial phase change. This phase change is actually beneficial because it allows the temperature profile of the coolant to stay relatively constant after reaching the boiling

temperature of 100 °C. As a result, the thermal driving force is nearly constant throughout the reactor.

For a single pass shell and tube plug flow reactor, thermal fluid can be run through the reactor co-current or counter-current with the feed stream. For this reaction, the thermal fluid runs co-current with the feed stream. The reactor initially drops in temperature, but then rises as the reaction proceeds. If the thermal fluid is fed in to the reactor co-currently, the thermal driving force (or temperature difference between the two fluids) is maintained at a larger average value. When the thermal coolant is run counter-currently, the thermal driving force is larger at the hotspot, but does not allow the reactor to maintain an appropriate temperature range for the length of the reactor.

Appendix B: Separation Process Design

Submitted to:

Dr. Jennifer Anthony

CHE 560

Submitted by:

Tristan Grieves, Nikki Klaassen, Patrick O'Connor, Sarah Keffer

November 20, 2015

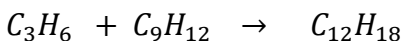
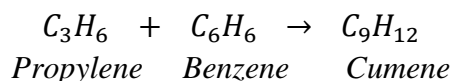
Appendix B: Separation Process Design

B.1 Executive Summary

In this process, cumene is produced through a reaction between propylene and benzene with p-diisopropylbenzene (DIPB) as a byproduct. Propane acts as an inert. Distillation selected as the primary method to separate cumene from the other three components. Three distillation columns in series were employed to purify the cumene product. These columns were sized in order to maximize stream purity while minimizing size and cost. The first column, Column 1, is fed the total mixture of the four components and separates benzene, propane, and propylene from the cumene and DIPB. In this column, benzene is treated as the heavy key and cumene as the light key. Column 1 is a trayed column containing 19 sieve trays with a height of 15.24 m and a diameter of 0.76 m. The distillate from Column 1 then enters Column 2. Column 2 separates propane and propylene from benzene. This is a low energy-intensive process so the column is small in comparison to the other two. Due to its small size, Column 2 is a packed column consisting of 4 equilibrium phases with a height of 5.48 m and a diameter of 0.31 m. The bottoms containing benzene at 96.4% purity are then recycled back into the reactor. The bottoms of Column 1, the stream containing cumene and DIPB, enters Column 3. This column separates the cumene at 99.5% purity from the DIPB at 98.6% purity. Both of these purities meet or exceed the requirements for sale. Column 3 is a trayed column containing 23 sieve trays with a height of 17.68 m and a diameter of 1.37 m. Other process designs were studied for this separation, most notably three columns with the bottoms of each feeding to the next column. Other methods of separation were explored, but were determined to be inappropriate for the necessary separation. It was determined that the chosen process could achieve the same purity at a lower overall cost, about \$3 million less over ten years in operating costs. This is mostly due to the small size of the second column as well as making this column packed instead of trayed. Overall equipment and equipment installation cost is estimated to be \$1.59 million. Operating costs for the separation process reach around \$1.38 million per year with an initial capital cost of \$6.54 million.

B.2 Introduction

The goal of this design process is to produce cumene product at 100,000 metric tons per year with a purity of at least 99.5 mol%. The mechanism for production of cumene in this process is by the Friedel-Crafts alkylation of benzene with propylene. A secondary reaction involved in this process is the formation of a byproduct, p-diisopropylbenzene (DIPB), from propylene and cumene. If the purity of DIPB exceeds 98 mol%, the byproduct can be sold for profit.



The separation of cumene from this mixture involves a multistage distillation process. This appendix provides the detailed separation process for cumene purification, the approach behind the design, and an overall cost analysis for the separation portion of cumene production.

B.3 Design Approach

The separation of cumene from the mixture of benzene, propylene, propane, and DIPB requires a series of separation stages. This process uses three separate distillation columns. The order of these columns was determined with respect to the energy requirements of each separation as well as how these separations affect the size of each column. Ideally, the separation process achieves high separations while maintaining low operating and capital costs.

B.3.1 Design Comparison

The final distillation design shown in Figure 1 begins with feeding benzene, propylene, propane, cumene, and DIPB at exit reactor concentrations into Column 1. This column separates benzene, propane, and propylene from cumene and DIPB, treating benzene as the heavy key and cumene as the light key. The distillate of this separation feeds into a cooler, and then proceeds into Column 2, a small packed column that separates propane and propylene from benzene. The bottom stream of Column 1 feeds into Column 3, a distillation tower that separates the final product, cumene, from DIPB. This separation procedure is the final design because it produces market-quality cumene while maintaining low costs.

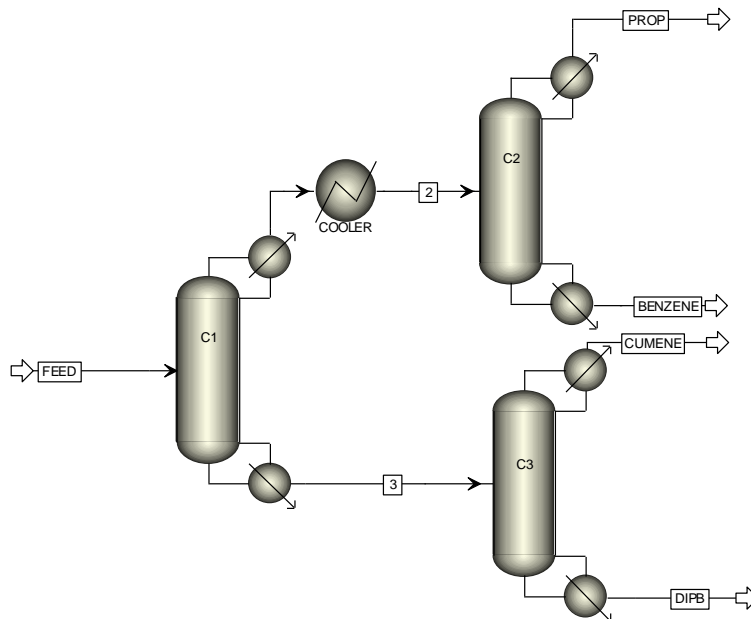


Figure 8. Separation process flow sheet

The original base case for this process includes a column separating the lightest components of the feed mixture, propylene and propane, from the feed, leaving benzene, cumene, and DIPB in the bottoms. The bottoms mixture from the first column is then fed into a second distillation column to separate benzene from the cumene and DIPB. From there, the cumene and DIPB enters a third and final distillation column to achieve the finished products of cumene in the distillate and DIPB in the bottoms. When comparing this base case process to the approach in the final process, both designs achieve similar separations. However, the final design does so at a lower cost. This is primarily due to the small size of Column 2 when compared to any column in the base case design. The separation of propane and propylene from benzene with a low flow rate is a low energy-intensive process and thus does not require a large separation vessel to achieve the desired separation.

Another aspect of column design for this process was the means of separation: trays or packing. The final design includes one packed tower, Column 2, and two trayed towers. Similar separations and operating costs are achieved by trays and packing for all three columns, so the main consideration for each column was size. By convention, a column with a diameter of less than 0.61 m (2 ft) is too small for a worker to service the trays in the tower and packing must be used instead of trays. Column 2 in the final separations design has a diameter of 0.305 m, and is therefore suitable for using packing. Columns 1 and 3 are trayed because of their larger overall size. The diameters of both columns exceeds the minimum necessary for service within the column. Additionally, packing in a tower with a height greater than 6.1 m may cause liquid channeling. This leads to a reduction in contact because liquid flows down the sides of the column while gas flows up the center. Columns 1 and 3 are 15.24 and 17.68 m, respectively, making them too tall to sustain packing as the separation medium without liquid channeling concerns.

B.3.2 Separations Considered

Distillation separates a feed using the differences in volatilities of each component. Components with higher volatilities vaporize and exit the top of the column while components with lower volatilities exit the bottom as a liquid. Distillation is chosen for this design because of the differences in boiling points among the components in the feed. Propane and propylene have the highest volatility, followed by benzene and then cumene. DIPB is the heaviest component.

Multiple separation types were considered for the purification of cumene before settling on distillation. Absorbing and stripping columns transfer a target compound from the gas phase to the liquid phase and vice versa. This technique only moves the target compound, cumene, into another material. This would necessitate another column to separate the cumene from another material. This technique also requires a large difference in volatilities between the target compound and the rest of the stream, which is not true for cumene, benzene, and DIPB.

B.3.3 Design Optimization

To optimize each column, different parameters are run using sensitivity analysis on Aspen. A block parameter, such as distillate flow, is selected and varied while collecting exiting stream composition data. These compositions are evaluated by graphing them to visually determine the optimum distillate flow. This process is then repeated with reflux ratio, number of stages, and feed stage location. One example, Figure 2, shows the distillate flow for Column 1 was varied to determine the point where maximum benzene and minimum cumene would exit with the distillate.

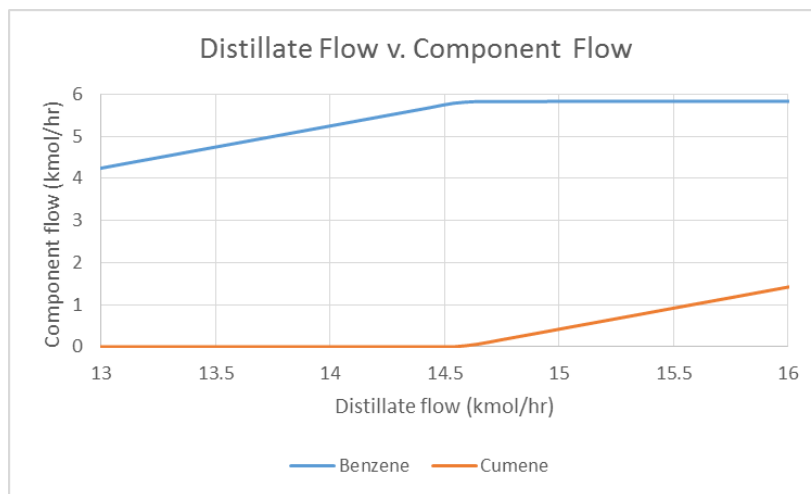


Figure 9. Sensitivity analysis to optimize distillate flow for Column 1. In this example, a flow rate of 14.6 kmol/hr was selected as the optimum point of operation because of the maximized benzene flow and minimized cumene flow.

B.3.4 Tray/Packing Sizing and Rating

The ideal design of individual tray and packing types for each column can depend upon a number of different factors. For both trayed columns, inexpensive sieve trays are selected as the tray of choice. The relative pressure drop in both trayed columns is not large enough to require the use of a more expensive tray. In addition, the columns are small enough that they have no need for the efficiency boost granted by such a tray. With the relatively small column area found in both columns, a single pass tray will be enough. When designing the tray rating, the Kister method is used as the primary flooding calculation model. The resulting downcomer area to column area ratio is 0.177 for Column 1 and 0.11 for Column 3. The efficiency rating for each tray is set to 70%. Finally, the resulting weir height for Columns 1 and 3 is 0.05 meters.

In the packed column, the tray height and diameter are both relatively small. As a result, the pressure drop is minimal and the separation fairly sharp. Thus a generic random plastic Pall ring is selected as the packing of choice, because the need for a more expensive type of random packing or structural packing is not present. The use of corrosive-resistant metals is not needed because of the relatively mild chemicals used in this process and the high cost of metal packing. The ring size is to be 25 mm to minimize liquid channeling by reducing packing size to less than one-eighth of the column diameter. The Eckert Generalized Pressure Drop Correlation, which is

appropriated for most generic random packing types, is used as the method to calculate pressure change throughout the column.

B.3.5 Aspen Analysis Model

The Soave-Redlich-Kwong (SRK) property method is used to solve this process in Aspen. It is a cubic equation of state and is used for nonpolar or mildly polar mixtures. This method is often used when dealing with hydrocarbons. The SRK method performs well in high temperature and pressure systems but gives reasonable results over all temperatures and pressures. These properties of the SRK method fit well with the cumene purification process.

B.4 Results

The final cumene separation design met the required purity of cumene at a final purity of 99.51 mol% as shown in Table 1 in reference to the flowsheet provided in Figure 2. Table 2 displays properties of each stream in the separation process. The final purity of DIPB was 98.6 mol%, just above the 98 mol% required purity needed to sell the byproduct. The purity of the benzene in the final benzene stream is 96.4 mol% benzene. This is pure enough to be recycled back into the process. The actual feed into Column 1 does not contain propylene because all of the supplied propylene is consumed in the reactor. Therefore, the second column only separates propane and benzene and no propylene exists anywhere in the separation streams.

Table 1. Stream table of separations process design showing composition percentages for each component. The feed stream refers to the stream entering Column 1, Stream 1 is the distillate of Column 1 while Stream 2 is the bottoms stream. Stream 1 enters a cooler and Stream 3 is the exiting cooled stream. The propane, benzene, cumene, and DIPB streams are the streams in which those components are the primary component.

Stream	Feed	1	2	3	Prop	Benzene	Cumene	DIPB
Benzene mol %	6.10	55.20	55.20	0.43	24.13	96.40	0.44	-
Propane mol %	4.48	43.25	43.25	-	75.87	-	-	-
Cumene mol %	86.89	1.55	1.55	96.76	-	3.60	99.51	1.42
P-DIPB mol %	2.52	-	-	2.81	-	-	0.05	98.58

Table 2. Stream table of separations process design results including component flow rates, component mole percentages, operating conditions and quality of each stream.

Stream	Feed	1	2	3	Prop	Benzene	Cumene	DIPB
Benzene (kmol/hr)	6.85	6.42	6.42	0.43	1.60	4.82	0.43	-

Propane (kmol/hr)	5.03	5.03	5.03	-	5.03	-	-	-
Cumene (kmol/hr)	97.52	0.18	0.18	97.34	-	0.18	97.30	0.04
P-DIPB (kmol/hr)	2.83	-	-	2.83	-	-	0.05	2.78
Total Flow (kmol/hr)	112.23	11.63	11.63	100.6	6.63	5.00	97.78	2.82
Temperature (°C)	180.00	130.50	80.00	200.00	92.00	152.90	236.40	303.7
Pressure (bar)	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.02
Vapor Quality	0.00	1.00	0.42	0.00	1.00	0.00	1.00	0.00

B.4.1 Column 1

Column 1 separates benzene, propane, and propylene from cumene and DIPB. The column design, laid out in Table 3, includes a height of 15.24 m and a diameter of 0.762 m. The height to diameter ratio is within the acceptable limits. The column requires 19 trays to obtain the necessary separation.

Table 3. Column 1 design parameters

Diameter (meters)	0.762
Height (meters)	15.24
Height-to-diameter ratio	20
Design pressure (barg)	6.793
Design temperature (°C)	265.7
Number of trays	19
Tray height (meters)	0.6096

As shown in Figure 3, the cumene mole fraction increases as the stages move down the column. As a heavier component, this is expected. The benzene, propylene, and propane mole fractions increase toward the top of the column, as is expected of the lighter components. DIPB has a very low mole fraction overall, but it does increase slightly near the bottom of Column 1.

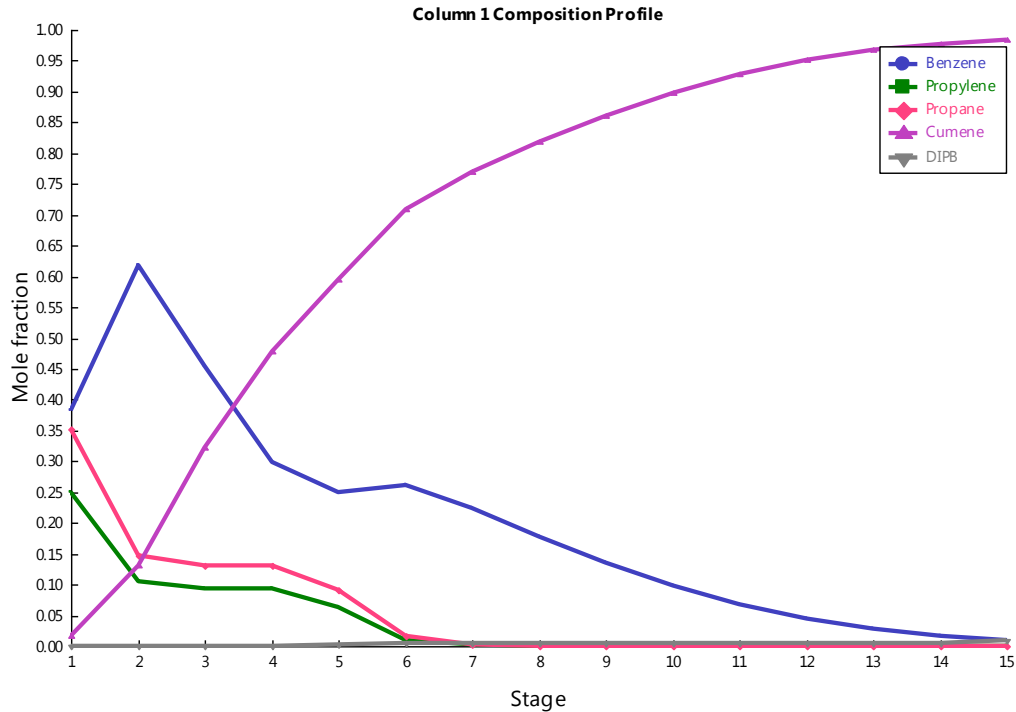


Figure 10. Column 1 composition profile by mole fraction and stage based on Aspen simulation

B.4.3

Column 2 separates propane and propylene from benzene, and is the only packed column in the design. The column design, laid out in Table 4, includes a height of 5.486 m and a diameter of 0.305 m. The height to diameter ratio is within the acceptable limits. The column requires 4 packed equilibrium stages to obtain the necessary separation.

Table 4. Column 2 design parameters

Diameter (meters)	0.305
Height (meters)	5.486
Height-to-diameter ratio	18
Design pressure (barg)	6.713
Design temperature (°C)	176.2
Number of equilibrium stages	4
Packing height (meters)	1.2192

Figure 4 details the composition in each equilibrium stage. Like in the trayed columns, the heavier components are more prominent in the bottom while the lighter components are more prevalent in the top of the column.

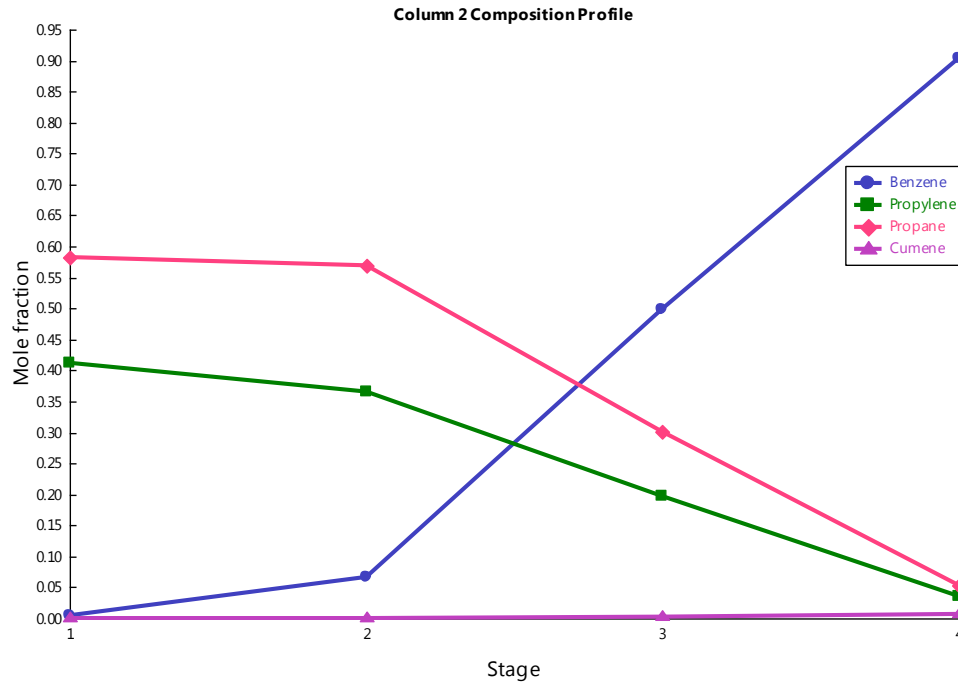


Figure 11. Column 2 composition profile by mole fraction and stage number based on Aspen simulation

B.4.3 Column 3

Column 3 separates the desired product, benzene, from DIPB. The column, with its parameters displayed in Table 5, has a diameter of 1.22 m and a height of 17.68 m. The height-to-diameter ratio is well under the maximum ratio of 20. The column is trayed and consists of 23 sieve trays.

Table 5. Column 3 design parameters

Diameter (meters)	1.219
Height (meters)	17.678
Height-to-diameter ratio	14.5
Design pressure (barg)	6.804
Design temperature (°C)	333.25
Number of trays	23
Tray height (meters)	0.6096

As can be seen in Figure 5, the lighter component, cumene, has a high mole fraction at the top of the column and the heavier component, DIPB, has a high mole fraction at the base of the column. This separation gives the final product at above the necessary purity.

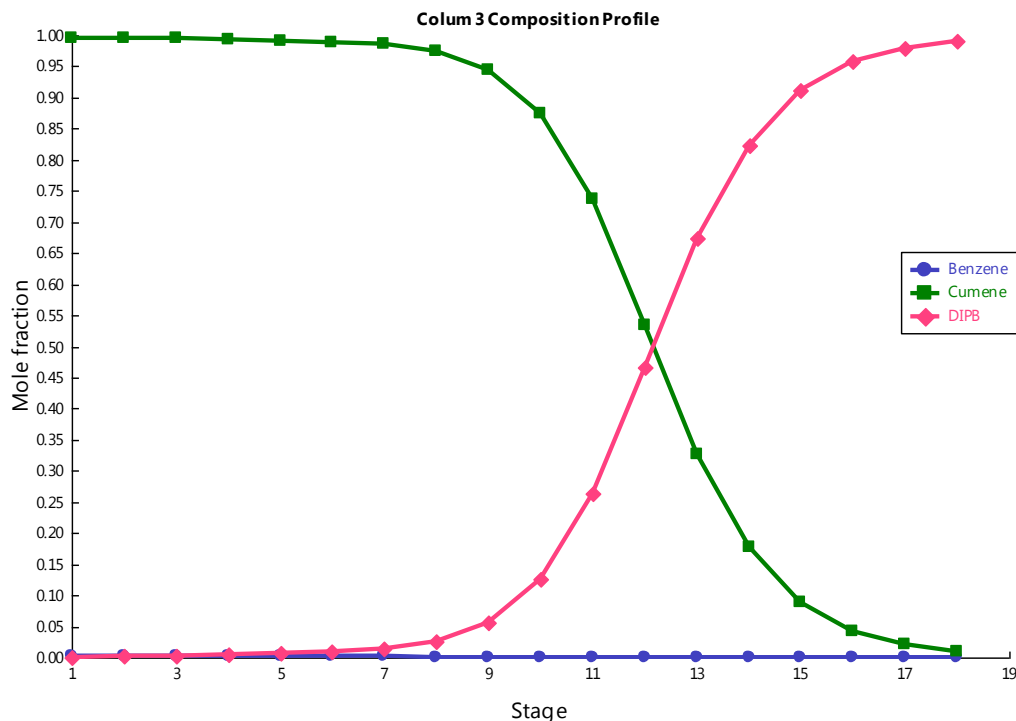


Figure 12. Column 3 composition profile by mole fraction and stage number based on Aspen simulation

B.5 Economic Analysis

While the purity of the final cumene product is the overall motivation for much of this design, another major factor in making design decisions was the cost. Both capital cost and utility cost were taken into consideration when choosing the order of separation, sizing the distillation columns, and picking trays and packing. The final design for cumene separation is the most cost effective over the 10 year planned life span of all the designs considered.

B.5.1 Economic Analysis of Three Design Configurations

The original base case design involves three columns in series to first distill propane and propylene from the mixture, followed by benzene, and finally cumene. The final selected design is modified so the first column separates propane, propylene, and benzene from cumene. This separation “splits” the flow into two streams, each to be separated by a different column. One of the final columns separates propane and propylene from benzene; and the second separates cumene from DIPB. Both design approaches achieve similar separation potential, but the resulting operating costs are much different. After further investigation, it was determined that the column that separates propane and propylene from benzene would need to be packed. The packed column results in an increased capital cost, but reduced operating cost. Both split column

approaches are far less costly than the base case design, and the series with a packed column proves to be most cost efficient long term (Table 5).

Table 6. Economic analysis of three design configurations

	Original series	Split series	Split series, 1 packed
Operating cost	\$1,628,050	\$1,389,970	\$1,376,500
Capital cost	\$7,008,540	\$6,425,310	\$6,541,120
Year 1	\$8,636,590	\$7,815,280	\$7,917,620
Year 2	\$10,264,640	\$9,205,250	\$9,294,120
Year 3	\$11,892,690	\$10,595,220	\$10,670,620
Year 4	\$13,520,740	\$11,985,190	\$12,047,120
Year 5	\$15,148,790	\$13,375,160	\$13,423,620
Year 6	\$16,776,840	\$14,765,130	\$14,800,120
Year 7	\$18,404,890	\$16,155,100	\$16,176,620
Year 8	\$20,032,940	\$17,545,070	\$17,553,120
Year 9	\$21,660,990	\$18,935,040	\$18,929,620
Year 10	\$23,289,040	\$20,325,010	\$20,306,120

B.5.2 Cost Impact of Design Parameters

Design parameters impact equipment costs in different ways. For example, increasing the number of trays can give a better separation, but can also increase the tower cost. As this and other parameters (reflux ratio, distillate flow rate, feed tray, etc.) are optimized, the capital and operating costs are considered in addition to separation potential. Column costs in this design vary greatly, from the small packed column, Column 1, to the large and energy-intensive cumene and DIPB separation in Column 3. While optimizing the packed column, it was determined that a lower feed temperature is necessary for an appropriate separation. In addition to providing a better separation, the inclusion of the cooler reduces the resulting size of Column 2, making it economically feasible.

Table 7. Cost breakdown of separation design equipment

	Column 1		Column 2		Column 3	
	Equipment cost	Installed cost	Equipment cost	Installed cost	Equipment cost	Installed cost
Condenser	\$8,600	\$59,600	\$8,500	\$65,100	\$8,600	\$60,200
Condenser accumulator	\$12,400	\$83,800	\$12,400	\$77,400	\$13,700	\$94,700
Reboiler	\$21,300	\$92,600	\$11,400	\$61,700	\$34,100	\$173,100

Reflux pump	\$4,400	\$32,200	\$4,400	\$25,900	\$5,500	\$40,300
Tower	\$67,600	\$234,600	\$15,000	\$125,300	\$109,200	\$307,600
SUBTOTAL	\$114,300	\$502,800	\$51,700	\$355,400	\$171,100	\$675,900
Cooler						\$51,700
TOTAL						\$1,585,800

B.6 Discussion

The final separations design for cumene production results in a cumene stream that exceeds the required purity. This is done using one packed column and two trayed columns in series. The design chosen minimized capital and utility costs while maximizing purity of cumene and DIPB. The design was also formed with safety and environmental impact in mind.

B.6.1 Interpretation of Results

Benzene and cumene are very similar compounds, both in physical shape and chemical properties. The separation of the two compounds takes first priority, and is the basis for Column 1. The column has a large feed flowrate and 15 total equilibrium stages. This comes out to be 19 trays after the efficiency is taken into consideration. Due to the large flow rate and height of the column from this many trays, the column diameter is also large, coming in at 0.762m, or 2.5ft. This gives a height-to-diameter ratio of 20.

The distillate composition of Column 1 contains all of the propane and propylene, almost all of the benzene, and a small amount of cumene. The distillate contains 95.5 mol% of the benzene from the feed, and the bottoms has 99.8 mol% of the cumene from the feed. This separation allows for almost all of the cumene to be recovered, and the remaining cumene will be recycled back into the reactor. This design allows for the highest separation without requiring higher energy costs to cool the feed stream by a significant amount.

Column 2 is designed to separate the propylene from the benzene. Propane and propylene are very similar, linear compounds, and are very different from the ring structure of benzene and cumene. The column also has a small feed stream, consisting of 14.5 kmol/hr total feed. The small feed and simple separation leads to a small column design, which in turn dictates a packed column. The column diameter was 0.305m (1ft), and the packed height was 1.22m (4ft). The small size allows for a much cheaper column than having a depropanizer column at the beginning of the distillation process, which would have required many more stages of trays or packing. The distillate of Column 2 contained almost exclusively propane and propylene, with only 0.5 mol% benzene. The bottoms of the column contained the benzene and all of the

cumene, with only 0.4 mol% propane and 0.3 mol% propylene in the stream. This allows for a nearly pure benzene recycle, and a distillate to be used as a fuel gas with little benzene impurity.

Column 3 was designed to separate the cumene from the DIPB. These two compounds are even more similar than cumene was to benzene, so the separation took more stages, and a larger column diameter. The final column had a diameter of 1.77m (4ft), a height of 17.7m (58ft), and had 23 trays. This gave the column a height-to-diameter ratio of 14.5.

The column produced a distillate containing 99.6 mol% cumene, with a bottoms containing 99.6 mol% DIPB. The cumene product has a 0.3 mol% benzene impurity, and a 0.1 mol% DIPB impurity. The DIPB product has a 0.4 mol% cumene impurity. Both streams produce chemicals with high enough purity to be sold.

B.6.2 Safety, Environmental, and Resource Conservation Issues

As with any chemical engineering process in the 21st century, safety and environmental considerations are as important as efficiency and profitability. The cumene production method used in this process fortunately does not involve any chemicals directly harmful to human or environmental health in small quantities. In addition, none of the chemicals are corrosive. However, nearly all compounds used are flammable. The separations portion of the process also uses some relatively high temperatures ($>300\text{ }^{\circ}\text{C}$) and high pressures ($>6\text{ bar}$). Thus, there are several items to be aware of when the separation process is being constructed. Any leaks presented in the separation process, or throughout the plant, must be spotted and eliminated to prevent a potential vapor cloud explosion. In the distillation columns themselves, care must be taken to ensure the columns are not operated near their structural limits. To account for this, it is recommended that pressure relief valves be installed at certain locations to prevent buildup. In addition, care was taken in designing the columns so that dry trays could be prevented. This further reduces the risk of vapor pressure buildup or overheating in the column. Finally, the columns were designed at a safe height-to-diameter ratio (20 or less) to prevent wind from having a potentially dramatic effect on the towers.

Reducing the environmental effect of the plant involves primarily reducing operational utilities, and therefore operational costs. When the columns were optimized, certain actions were taken in order to reduce utility usage as much as possible. For example, a heater between the first and third columns used in previous simulations was eliminated. This reduced the effectiveness of Column 3 in the separation, but was able to reduce utility usage dramatically. Several other tradeoffs were used in the optimization process to sacrifice a marginal increase in capital costs, but reduced utility and total costs in the long term.

In addition to reducing environmental effects by reducing utility cost, plant waste and recycle potential was also heavily considered in designing the columns. For instance, the purification of benzene (Column 2) was not necessary to separate cumene. However, since the cost of benzene

is relatively high, and because of the potential environmental impact of benzene as a volatile organic compound (VOC), the decision was made to include this process. In the final design of the plant, benzene can now be recycled back into the reactor. This will both reduce the intake of benzene into the plant and reduce the waste of benzene leaving. The separation of propylene from inert propane was also considered for recycle, but was determined to be not economically feasible for an additional column because of the relative difficulty of separation between propane and propylene.

Appendix C: Equations Employed in Economic Analysis

Pumps	$\log_{10}(\text{purchased cost}) = 3.4 + 0.05 \log_{10} W + 0.15 [\log_{10} W]^2$ $W = \text{power (kW, 1, 300)}$ assume 80% efficiency
Heat Exchangers	$\log_{10}(\text{purchased cost}) = 4.6 - 0.8 \log_{10} A + 0.3 [\log_{10} A]^2$ $A = \text{heat exchange area (m}^2\text{, 20, 1000)}$
Compressors	$\log_{10}(\text{purchased cost}) = 2.3 + 1.4 \log_{10} W - 0.1 [\log_{10} W]^2$ $W = \text{power (kW, 450, no limit)}$ assume 70% efficiency
Fired Heater	$\log_{10}(\text{purchased cost}) = 3.0 + 0.66 \log_{10} Q + 0.02 [\log_{10} Q]^2$ $Q = \text{duty (kW, 3000, 100,000)}$ assume 80% thermal efficiency
Horizontal Vessel	$\log_{10}(\text{purchased cost}) = 3.5 + 0.38 \log_{10} V + 0.09 [\log_{10} V]^2$ $V = \text{volume of vessel (m}^3\text{, 0.1, 628)}$
Packed Tower	Cost as vessel plus cost of packing
Packing	$\log_{10}(\text{purchased cost}) = 3 + 0.97 \log_{10} V + 0.0055 [\log_{10} V]^2$ $V = \text{packing volume (m}^3\text{, 0.03, 628)}$
Tray Tower	Cost as vessel plus cost of trays
Trays	$\log_{10}(\text{purchased cost}) = 3.3 + 0.46 \log_{10} A + 0.37 [\log_{10} A]^2$ $A = \text{tray area (m}^2\text{, 0.07, 12.3)}$

FCI = F_{Lang} * total equipment cost

Working capital = 17.5% of FCI

Cost of Labor = \$59,580 * number of operators

Supervisors and clerical employees = 17.5% of cost of labor

Maintenance and repairs = 6% of FCI

Operating supplies = 0.9% of FCI

Laboratory work = 15% of cost of labor

Catalyst cost = \$2.25/kg * catalyst loading * density of catalyst * volume of reactor

Plant overhead = 70.8% of cost of labor + 3.6% of FCI

Administrative costs = 17.7% of cost of labor + 0.9% of FCI