DESIGN OF CUMENE PLANT USING ASPEN PLUS

A Thesis

By

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Under the guidance of
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CERTIFICATE

This is to certify that the thesis entitled, "**Design of Cumene Plant using Aspen Plus**" submitted by **Krishna Tewari** for the requirements for the award of Bachelor of Technology in Chemical Engineering at National Institute of Technology Rourkela, is an authentic work carried out by him under my supervision and guidance.

To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other University / Institute for the award of any Degree or Diploma.

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Krishna Tewari

ABSTRACT

The work deals with optimization of the process of production of cumene from benzene by its alkylation with propylene. This process also involves an undesirable reaction between cumene and propylene to form p-diisopropylbenzene (PIDB). Since the activation energy of the second reaction is higher than the first one, lower reactor temperature is favored to improve the selectivity of the reaction towards cumene. This can be done by increasing the reactor size, finding a suitable method of distillation and designing the distillation columns accordingly. All the variations increase the capital and/or energy cost but also decrease the amount of raw material required. Thus this provides a classic example of an engineering design and optimization of a process. The process present in the design book by Turton et. al is referred and consists of a tubular reactor and two distillation columns. The purpose of this project is to develop an optimum design for the cumene plant which is aimed at saving maximum amount of raw material possible and also reduce the costs to an extent.

Keywords: Optimization, Simulation, Cumene, Benzene, Distillation

CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

1. INTRODUCTION:

The process considered for studying in this report is the production of isopropyl benzene, popularly known as cumene from benzene in a cumene production plant. This process is a classic example to study trade-off in engineering design and simulation as it has a lot of scope for optimization in the reaction section of the plant and the cost in the separation section.

Cumene is produced by the reaction of propylene and benzene and it also involves an undesirable reaction between cumene and propylene to produce p- diisopropylbenzene(p- DIPB). The raw materials fed to the plant are benzene and propylene with a small amount of propane as impurity in propylene. The process description of Turton et al. (2003) has been utilized which provides relevant and valuable data required for the simulation of the process.

1.1. Industrial Uses of Cumene:

Around 98% of cumene is used to produce phenol and its co-product acetone. It is used as feed back in the process. The cumene oxidation process for phenol synthesis has been growing in popularity since the 1960's and is prominent today. The first step of this process is the formation of cumene hydroperoxide. The hydroperoxide is then selectively cleaved to Phenol and acetone. The largest phenol derivative is bisphenol-A (BPA) which supplies the growing polycarbonate (PC) sector. PC resins are consumed in automotive applications in place of traditional materials such as glass and metals. Glazing and sheet uses, such as architectural, security and glazing outlets, are also important PC applications. The third largest use for PC is optical media such as compact discs (CDs) and digital versatile discs (DVDs). [Schmidt et. al, 2002]

Cumene in minor amounts is used as a thinner for paints, enamels and lacquers and to produce acetophenone, the chemical intermediate dicumylperoxide and diisopropyl benzene. Cumene is also used as a solvent for fats and raisins.

1.2. Objective of the Project:

Considering the amount of designing possible in this process, work was undertaken to develop the economically optimum design considering production rate, reactor design, capital costs, energy costs, and raw material costs. The objectives of the current project are as following:

- To use the cumene process to illustrate the process design optimization features using the optimization variables reactor size and benzene recycle ratio.
- To develop an optimum design to achieve a low capital cost, low operating cost and an appreciable conversion rate of reactant to products.

CHAPTER 2

LITERATURE

REVIEW

2. LITERATURE REVIEW

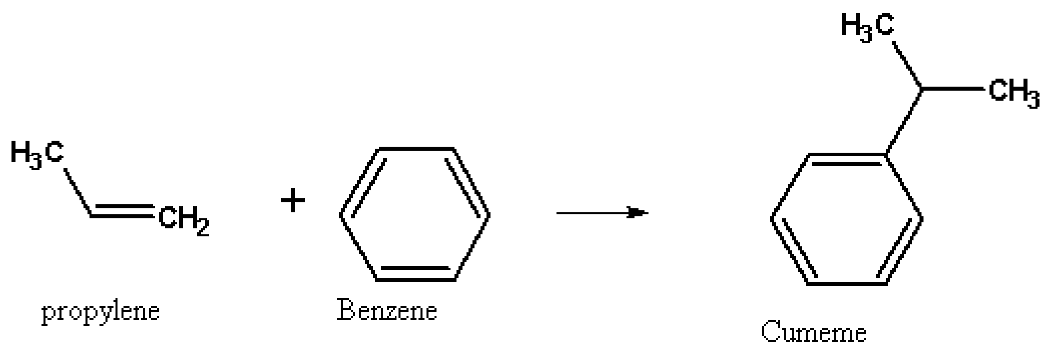
2.1. Process:

The process of production of cumene usually involves alkylation of benzene with iso-propylene catalyzed by various catalysts like zeolites, protonic acids (H_3PO_4) or lewis acids (BF_3) on various supports like amorphous or crystalline aluminosilicates. The two processes most widely used are UOP's Cumox process; which uses mixture of propylene and excess benzene reacted in the presence of solid phosphoric acid as a catalyst. The process offers 99.3% (byweight) conversion of propylene with 92.5% selectivity to cumene and UOP's Moonsanto- Lummus process; which involves mixing of dry benzene and propylene in alkylation reactor with $AlCl_3$ catalyst. The processes documented have many drawbacks like high catalyst volume, high reaction temperature, high feed mole ratio, lower yield, by-product formation etc. [Bokade and Kharul, 2009].

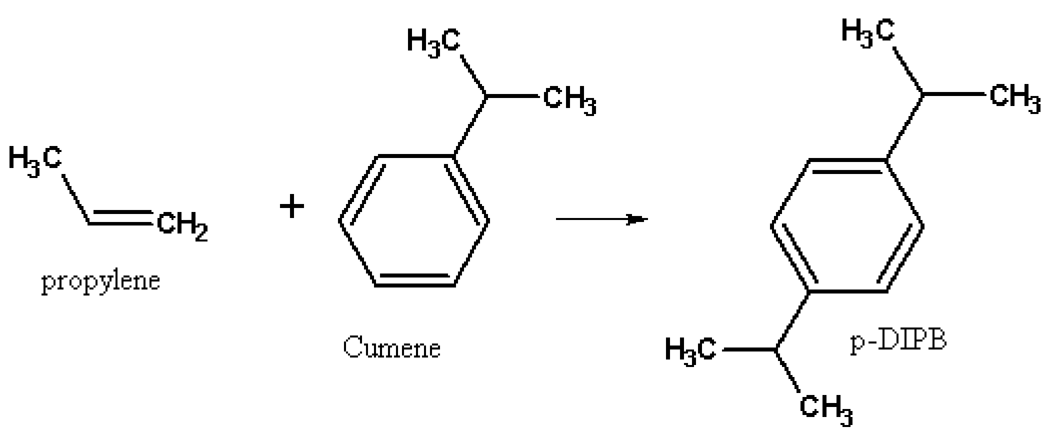
The most commonly used reactor in the industries is fixed bed reactor, which is easy to be implemented. In the process generally used, the feeding molar ratio must be large enough to maintain the catalyst activity run for a long time. [Lei et. al, 2009]

2.2 Reaction Mechanism and Kinetics:

The production of cumene from benzene involves the reaction of benzene with propylene in a high temperature, high pressure gas-phase reactor.



This is followed by another reaction in which cumene reacts with propylene to form p-diisopropylbenzene (PDIB). [Ding and Fu, 2005].



The reactions occur in vapor phase in the presence of a catalyst of solid density 2000kg/m^3 and 0.5 void fraction). The kinetic data and the reaction conditions specified by Turton et al (2003) for a particular catalyst have been used in the present work.

Table 5: Kinetic data of the reactions

	Reaction 1	Reaction 2
K	2.8×10^7	2.32×10^9
Activation Energy (KJ/kmol)	104174	146742

Since the activation energy of the undesirable reaction is more than that of the desirable reaction, lower reactor temperatures improve selectivity. In addition selectivity is improved by keeping the concentration of cumene and propylene low in the reactor. [Turton et. al, 2003].

Process Flowsheet:

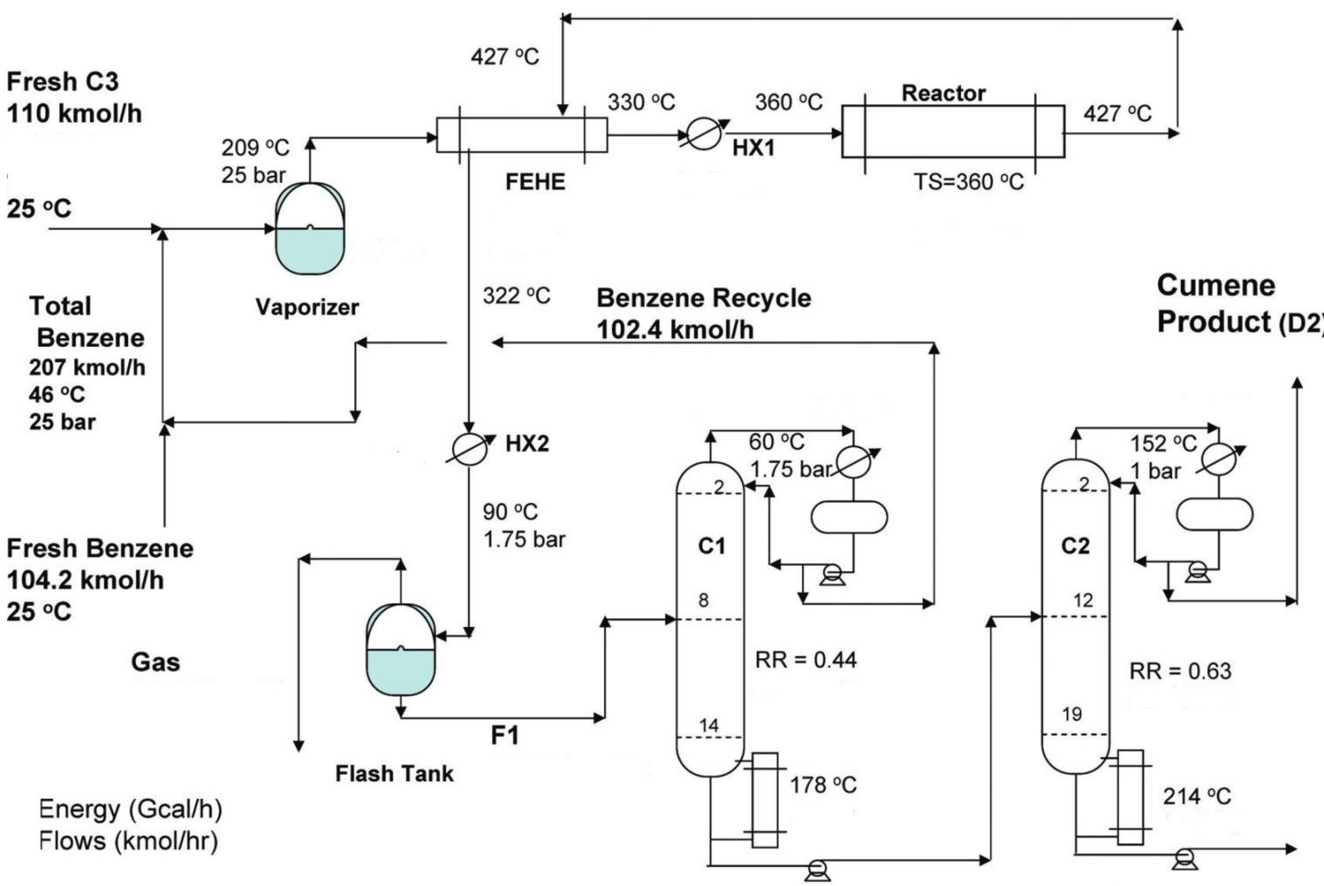


Figure 1: Process Flowsheet [Luyben, 2010]

2.3. Process Description:

Fresh feed streams of benzene and mixed C3(propylene and propane) enter the process as liquids at 110kmol/hr. Composition of this feed is 95 mol% propylene and 5 mol% propane. Since propane doesn't react, it is vented in the gases from the flash tank. Fresh feed of benzene is introduced at 104.2kmol/hr. The liquid fresh feeds are combined with benzene recycle stream and fed to the vaporizer. The total benzene fed to the reactor is 207 kmol/hr. Saturated gas leaves the vaporizer at 209°C and 25bar. It is preheated in two heat exchangers. First recovers heat from the reactor and the second adds heat to bring the reactor inlet temperature to 360°C.

The reactor is a cooled reactor filled with solid catalyst. Temperature on the steam side of the reactor is 360°C. The reactor inlet temperature is assumed to be set to the same value as coolant(steam) temperature in the reactor. Reactor effluent leaves at 427°C, which is cooled to 322°C in feed-effluent heat exchanger and sent to a condenser where it is again cooled to 90°C. The two phase stream is then sent to flash tank in which the gases separated out are used as fuel and the liquid from the bottom is sent to the benzene column.

The benzene column consists of 15 stages and fed on the 6th stage which is the optimum feed stage to minimize reboiler heat input. Operating pressure is 1.75 bar and cooling water is used in condenser. Distillate is mostly benzene and is recycled back to the reactor. Design specification is to keep the benzene from coming out of bottom and affecting the quality of cumene leaving from downstream which is then sent to the cumene column.

The second distillation column consists of 20 stages and is fed on stage 12 with an operating pressure of 1bar. Design specification is to attain high purity cumene in distillate and minimize loss of cumene in bottoms. Undesired byproduct containing mostly PDIB leaves from the bottom.

CHAPTER 3

PROCEDURE, RESULT & DISCUSSION

3. PROCEDURE, RESULT AND DISCUSSION:

3.1 Procedure:

The process described above was simulated in the Aspen Plus simulation software and the results obtained were studied. The design proposed by Turton et. al. was used for reference and the required data like inlet feed rate, inlet temperature, pressure, size of the reactor, reflux ratio and no. of stages in the distillation columns, properties of the catalyst etc were input. The Turton design was taken as the base run and all the parameters optimized were compared to the result obtained from the base run.

The process is mainly divided into a Reaction section and a Separation section. The optimization process mainly involves designing both the sections to get the most economical output. So it involves design of the reactor in reaction section and design of flash tank, benzene column and the cumene distillation column in the separation section.

In the Aspen Plus software, NRTL physical property package was chosen for the calculations. The blocks most suitable for the process were chosen from the available options to give the best results. Shell and tube heat exchangers were chosen for the feed effluent heat exchanger. The flowsheet of the process designed using aspen plus and the results obtained from the base run are as following:

Heat and Material Balance Table

Stream ID		PRODUCT	BYPRODCT	GASES	BYPRODCT	CLM1FEED	CLM2FEED	FEHEFEED	FLTNKFED	FRSHBNZN	GASES	PRODUCT	PRPLN	RCCLBNZN	RCTRFEED	RCTRPRDC
From		CUMNCLM	CUMNCLM	FLSHTNK	CUMNCLM	FLSHTNK	BNZNCLM	VAPORIZR	HX2		FLSHTNK	CUMNCLM		BNZNCLM	HX1	REACTOR
To						BNZNCLM	CUMNCLM	FEHE	FLSHTNK	VAPORIZR			VAPORIZR	VAPORIZR	REACTOR	FEHE
Phase		LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	VAPOR	VAPOR	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID
Substream : MIXED																
Mole Flow	kmol/hr															
PROPY-01		0.0	0.0	0.0	0.0	0.0	0.0	104.5000	0.0	0.0	0.0	0.0	104.5000	0.0	104.5000	0.0
PROPA-01		0.0	0.0	5.499779	0.0	.4168628	5.2770E-18	5.916863	5.916643	0.0	5.499779	0.0	5.500000	.4168628	5.916863	5.916643
BENZE-01		8.57897E-6	8.1050E-21	6.753527	8.1050E-21	13.85477	8.57897E-6	118.0548	20.60835	104.2000	6.753527	8.57897E-6	0.0	13.85476	118.0548	20.60835
P-DII-01		.7893121	6.240299	.0426377	6.240299	7.030581	7.029612	9.69040E-4	7.073203	0.0	.0426377	.7893121	0.0	9.69040E-4	9.69040E-4	7.073203
ISOPR-01		82.11757	3.87119E-6	8.254353	3.87119E-6	163.6505	82.11757	81.53290	171.9048	0.0	8.254353	82.11757	0.0	81.53290	81.53290	171.9048
Total Flow	kmol/hr	82.90689	6.240303	20.55030	6.240303	184.9527	89.14719	310.0055	205.5030	104.2000	20.55030	82.90689	110.0000	95.80549	310.0055	205.5030
Total Flow	kg/hr	9998.148	1012.645	1769.109	1012.645	21911.37	11010.79	23679.97	23680.47	8139.441	1769.109	9998.148	4639.958	10900.57	23679.97	23680.47
Total Flow	l/min	205.7489	21.87774	32800.81	21.87774	456.4337	234.9756	20222.43	13230.53	155.5573	32800.81	205.7489	152.4355	223.1404	10879.58	1408.579
Temperature	K	354.2302	404.8352	363.1500	404.8352	363.1500	386.0990	482.1500	836.2877	298.1500	363.1500	354.2302	298.1500	346.2560	633.1500	700.1500
Pressure	atm	.0986923	.0986923	.3111565	.0986923	.311571	.296070	10.10829	17.76462	24.67308	.3111565	.0986923	24.67308	.2960770	24.67308	24.67308
Vapor Frac		0.0	0.0	1.000000	0.0	0.0	0.0	1.000000	1.000000	0.0	1.000000	0.0	0.0	0.0	1.000000	0.0
Liquid Frac		1.000000	1.000000	0.0	1.000000	1.000000	1.000000	0.0	0.0	1.000000	0.0	1.000000	1.000000	1.000000	0.0	1.000000
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-7056.800	-23850.87	2002.016	-23850.87	-5662.458	-6602.161	14258.51	33073.21	11733.75	2002.016	-7056.800	-67.70048	-4390.946	20133.28	23106.78
Enthalpy	cal/gm	-58.51657	-146.9782	23.25579	-146.9782	-47.79651	-53.45338	186.6647	287.0147	150.2138	23.25579	-58.51657	-1.604983	-38.59217	263.5741	200.5244
Enthalpy	cal/sec	-1.6252E+5	-41343.52	11428.34	-41343.52	-2.9091E+5	-1.6349E+5	1.22784E+6	1.88796E+6	3.39627E+5	11428.34	-1.6252E+5	-2068.626	-1.1685E+5	1.73373E+6	1.31903E+6
Entropy	cal/mol-K	-124.7965	-186.6500	-62.90266	-186.6500	-119.3914	-124.2771	-43.78520	-49.22812	-60.33300	-62.90266	-124.7965	-51.36273	-114.2255	-35.00475	-65.11290
Entropy	cal/gm-K	-1.034840	-1.150209	-.7306891	-1.150209	-1.007777	-1.006191	-.5732124	-.4272096	-.7723748	-.7306891	-1.034840	-1.217662	-1.003932	-.4582634	-.5650603
Density	mol/cc	6.71586E-3	4.75392E-3	1.04420E-5	4.75392E-3	6.75354E-3	6.32315E-3	2.55496E-4	2.58875E-4	.0111641	1.04420E-5	6.71586E-3	.0120269	7.15584E-3	4.74904E-4	2.43156E-3
Density	gm/cc	.8098987	.7714421	8.98915E-4	.7714421	.8000931	.7809884	.0195162	.0298305	.8720734	8.98915E-4	.8098987	.5073138	.8141788	.0362758	.2801934
Average MW		120.5949	162.2749	86.08677	162.2749	118.4701	123.5125	76.38565	115.2318	78.11364	86.08677	120.5949	42.18143	113.7782	76.38565	115.2318
Liq Vol 60F	l/min	192.8196	19.78550	37.21599	19.78550	422.6135	212.6051	512.5327	459.8295	153.7108	37.21599	192.8196	148.8135	210.0084	512.5327	459.8295

3.2 Reactor Design:

The reactor chosen for the process was a tubular high pressure and temperature reactor as prescribed in the Turton design. The feed stream contains benzene, propylene and propane (as inert) mainly. The size of the reactor was varied by varying the number of tubes in the reactor. The outlet flow rate from all the streams like the product, byproduct and the gases stream was kept constant and the amount of cumene present in the streams were monitored to analyze the results. Fresh propylene stream contains propane as impurity which is inert in the reaction. Since the separation of propylene and propane is difficult, economics favor designing reactor for high conversion of propylene. The undesirable byproduct is also burned. So it only has value as a fuel. Since it takes reactants to produce this product, there is a strong requirement to keep its production rate small.

To study the changes in the process by variation of reactor size, the number of tubes in the reactor was varied from 342(as in Turton design) to 1000. A larger reactor has both advantages and disadvantages. On one hand it increases the capital and/or energy costs and on the other hand it maintains low reactor temperature which improves the selectivity and reduces the production of PIDB [Lei et. al, 2007]. This in turn, saves raw material used which is given more preference in the design process. The result obtained after varying the reactor size is given below:

Table 6: Variation in Reactor Size

no. of tubes	%cumene in product	%cumene in Byproduct	%cumene in gases
342	99.0478	6.20323E-05	40.1663
350	99.0572	6.20002E-05	40.1030
370	99.1134	6.19842E-05	40.0938
390	99.1695	6.19361E-05	39.9755
410	99.2223	6.1856E-05	39.9502
450	99.3200	6.17919E-05	39.8295
470	99.3436	6.17759E-05	39.7475
490	99.3922	6.17118E-05	39.7059
510	99.4895	6.16958E-05	39.5653
530	99.5256	6.16477E-05	39.4164
550	99.5954	6.16156E-05	39.3882
570	99.6197	6.15996E-05	39.3317
590	99.6843	6.15676E-05	39.2957
610	99.7231	6.15515E-05	39.2028
630	99.7531	6.15035E-05	39.1619

700	99.8551	6.14554E-05	38.8826
750	99.8503	6.14073E-05	38.7653
800	99.8512	6.13592E-05	38.6879
850	99.8610	6.13432E-05	38.6286
900	99.8702	6.12791E-05	38.5298
950	99.8739	6.12631E-05	38.4948
1000	99.8733	6.12631E-05	38.0023

After the results were obtained, the percentage cumene present in the product, its percentage in the byproduct and the vent gases were plotted against the no. of tubes of the reactor to analyze the data. The graphs obtained are as following:

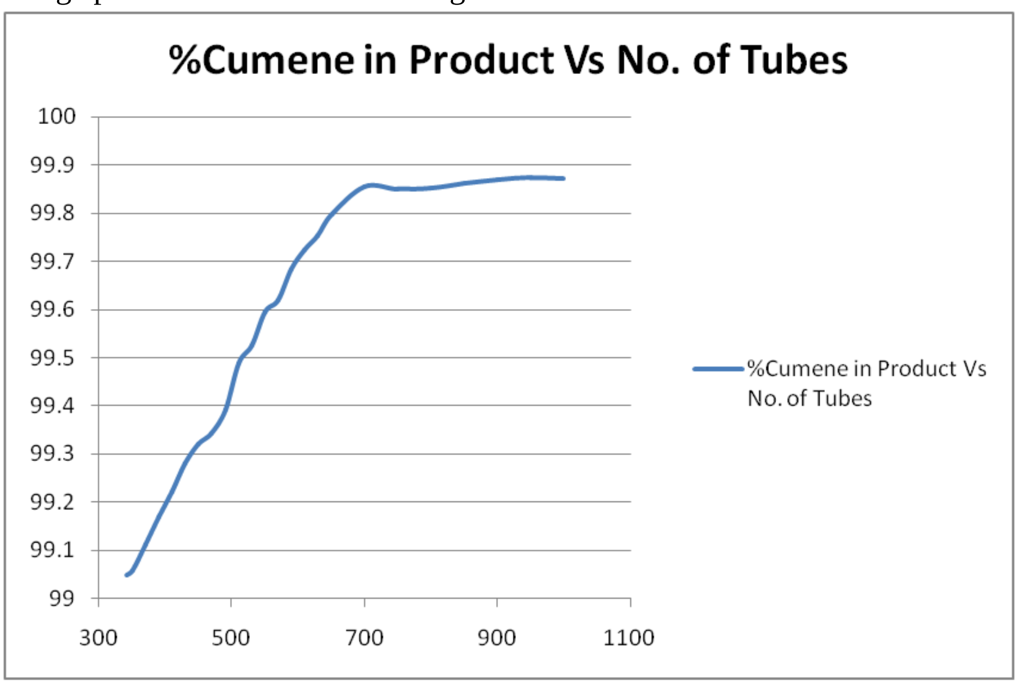


Figure 2: % Cumene in Product Vs Size Of Reactor

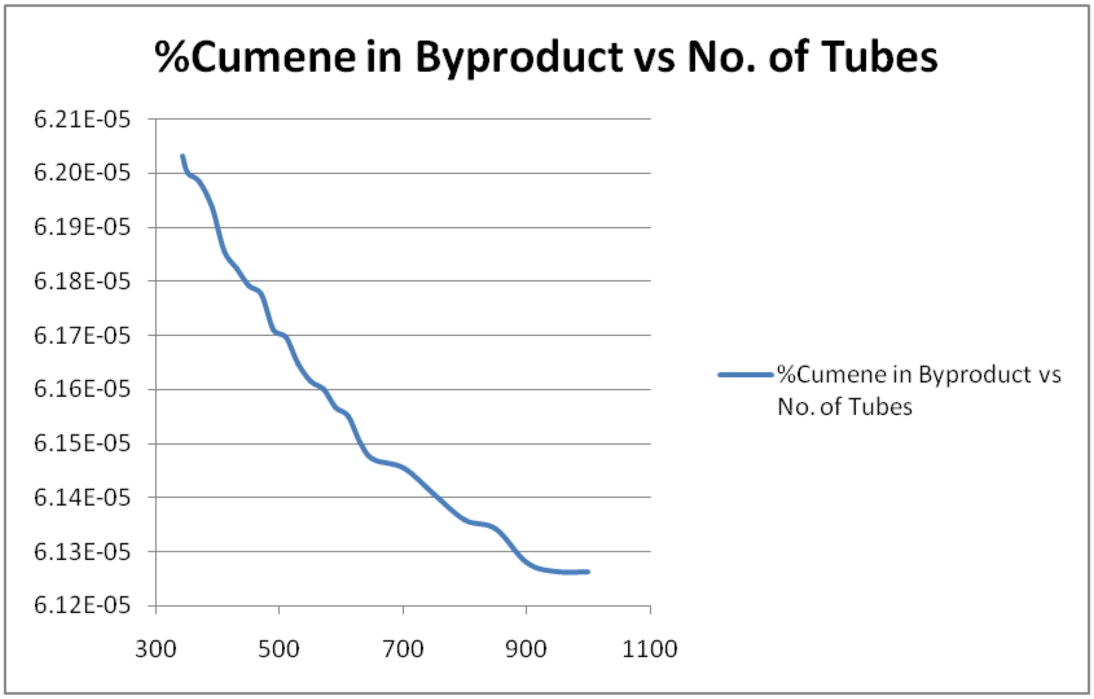


Figure 3: %Cumene in Byproduct Vs Size Of Reactor

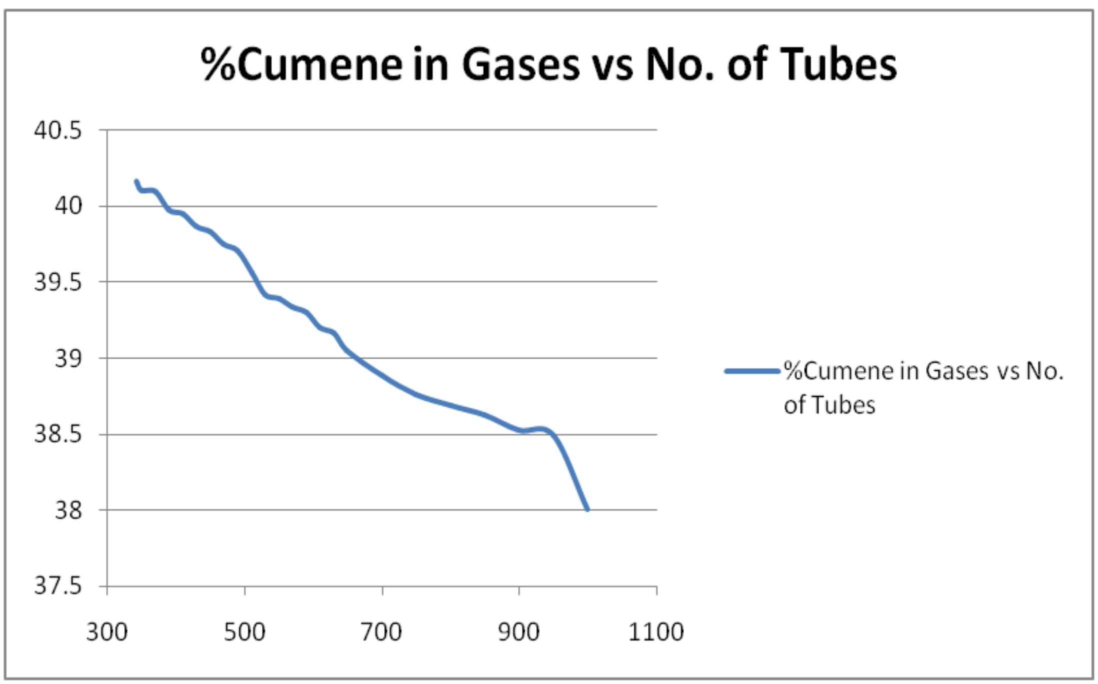


Figure 4: %Cumene in Gases Vs Size Of Reactor

We see that the as the number of tubes were increased, the amount of cumene in product stream kept on increasing and after a certain point, the rate of increase of cumene started decreasing. At the same time, the percentage of cumene present in the byproduct and gases from the flash tank decreased with increase in the size of the reactor.

Therefore, increase in the reactor size does increase the cumene production in the process. This saves a lot of raw material required for the production. Although the increase in reactor size calls for an increase in capital and/or energy investment but the amount of raw material it saves in the process is appreciable. It also reduces the amount of cumene present in the byproducts and the vent gases which is a great positive sign for considering this variation for optimizing the process. It might not even compensate for the extra capital investment but it may also turn out to be more profitable, considering the shortage of raw materials present in the present day scenario.

3.3 VLE Characteristics:

In the cumene plant, as the separation process plays a major role and involves considerable costs, it has to be optimized so as to make it as economic as possible. Since it consists of two distillation columns namely, the benzene and the cumene distillation column, its VLE (Vapor Liquid Equilibrium) characteristics have to be monitored accordingly so as to decide upon the method and type of distillation. When a fat curve is observed in the plot between two components, it means that they can be easily separated. The Txy diagram for Benzene-Cumene and the Cumene-DIPB systems have been plotted below. The boiling point of the benzene, cumene and DIPB are 80.2, 152.4 and 209.8°C respectively. The NRTL physical property package in Aspen plus software is used to plot the Txy diagram for all the components.

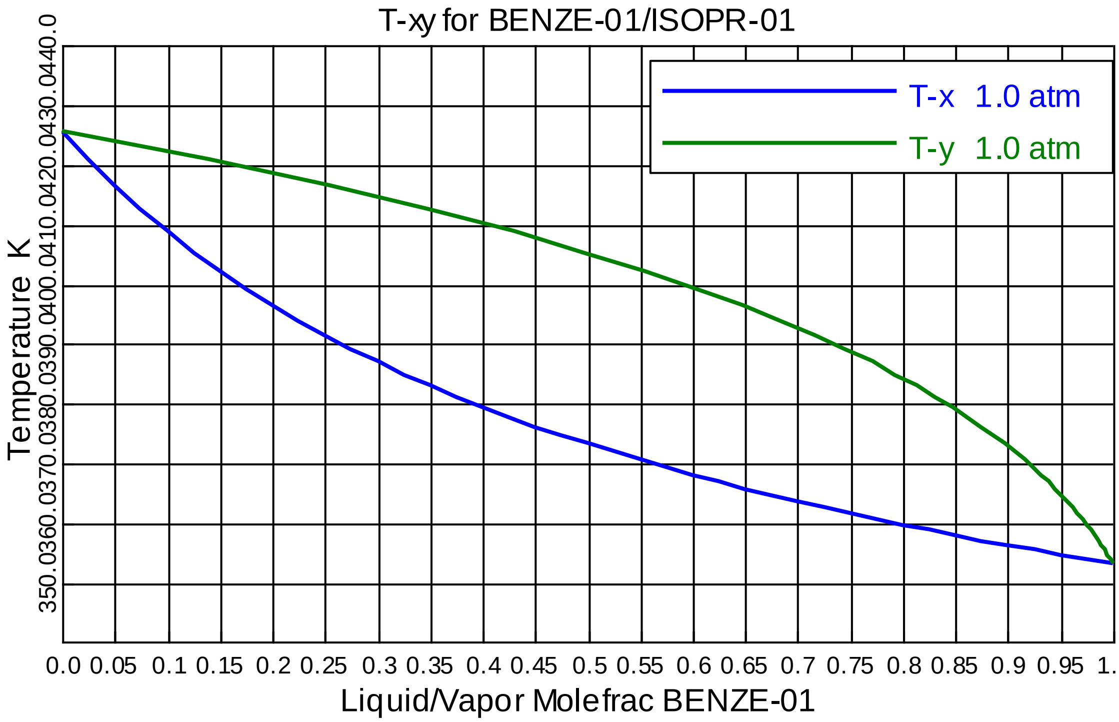


Figure 5: T-xy Diagram for Benzene-Cumene system

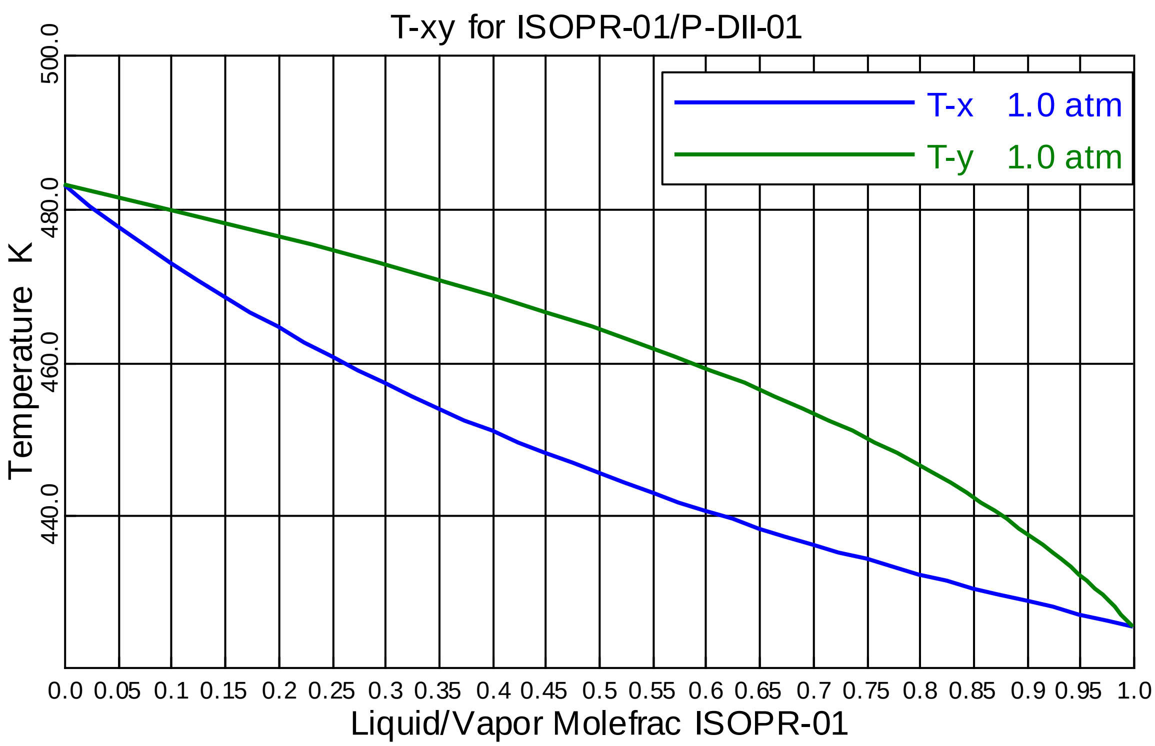


Figure 6: T-xy Diagram for Cumene-DIPB System

As seen from the above plots, an azeotrope is not formed in the plot. As the curve formed in both the cases is wide, it can be said that the separation in both the distillation columns would be easy and a low value of reflux ratio and lesser number of trays will be required.

3.3 Flash Tank Design:

A flash tank is installed in the system to flash the light vapors present in the outlet from the reactor. These vapors usually contain unreacted propylene and propane (as inert), which are used as fuel later on. Main purpose of installing a flash tank in the process is to vaporize the lighter components so that energy can be saved in the distillation columns and separation process can be easier.

In the Turton design, the flashing temperature is taken as 90°C. Since the minimum boiling point in the mixture is that of benzene, i.e. 80.2°C at 1 atm, the temperature was varied from 85 to 95°C. The pressure in the flash tank was set at 1.75 bar and the NRTL property package was utilized to calculate the data. The percentage of cumene present in the product and by-product streams from the cumene column and in the vent gases from the flash tank were used as parameters to check for the optimized results. After the results were obtained from the simulations, 3 graphs were plotted between the 3 parameters and the flashing temperature to analyze the results.

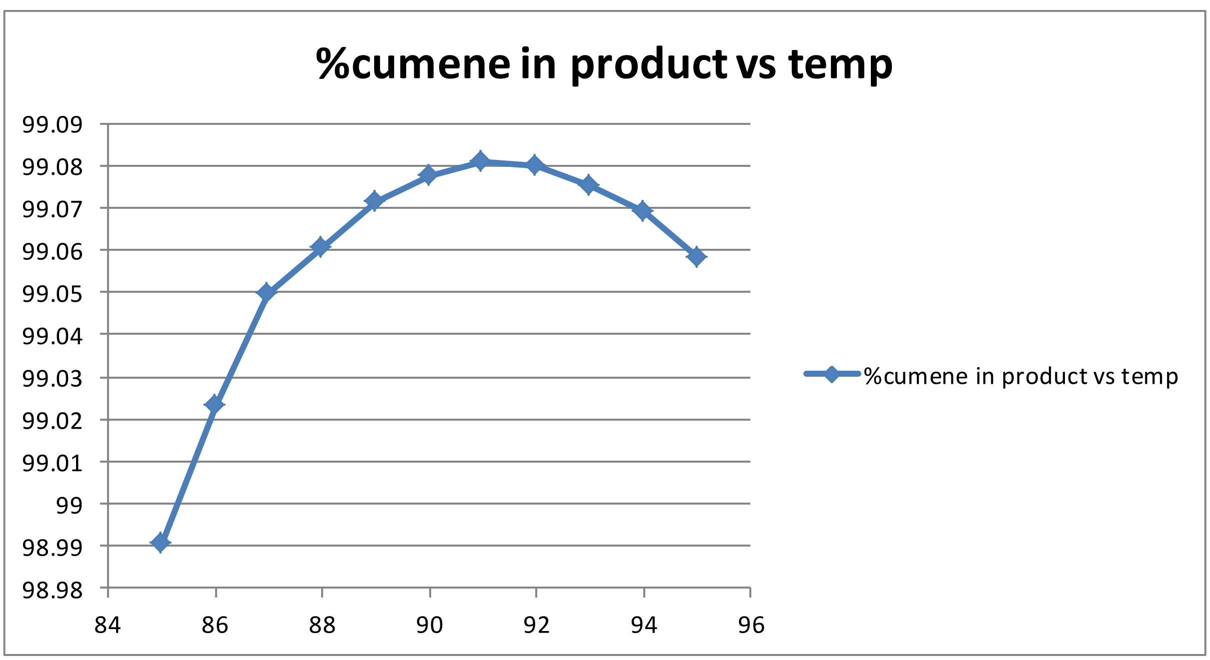


Figure 6: %Cumene in Product Vs Flashing Temperature

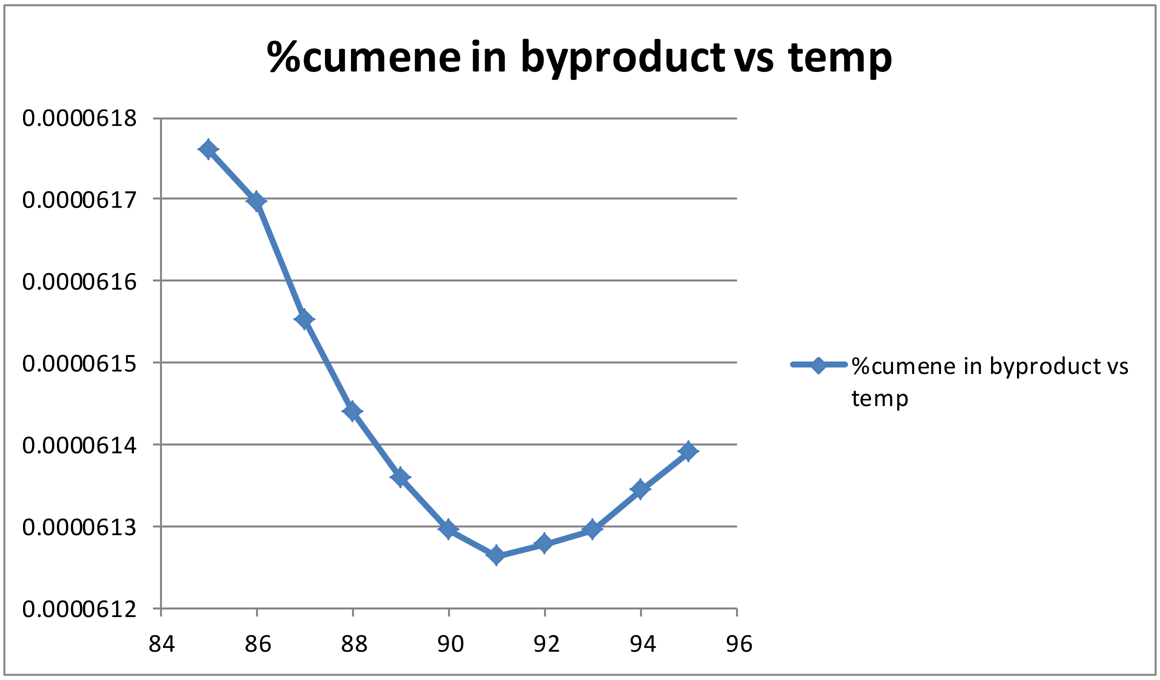


Figure 7: %Cumene in Byproduct Vs Flashing Temperature

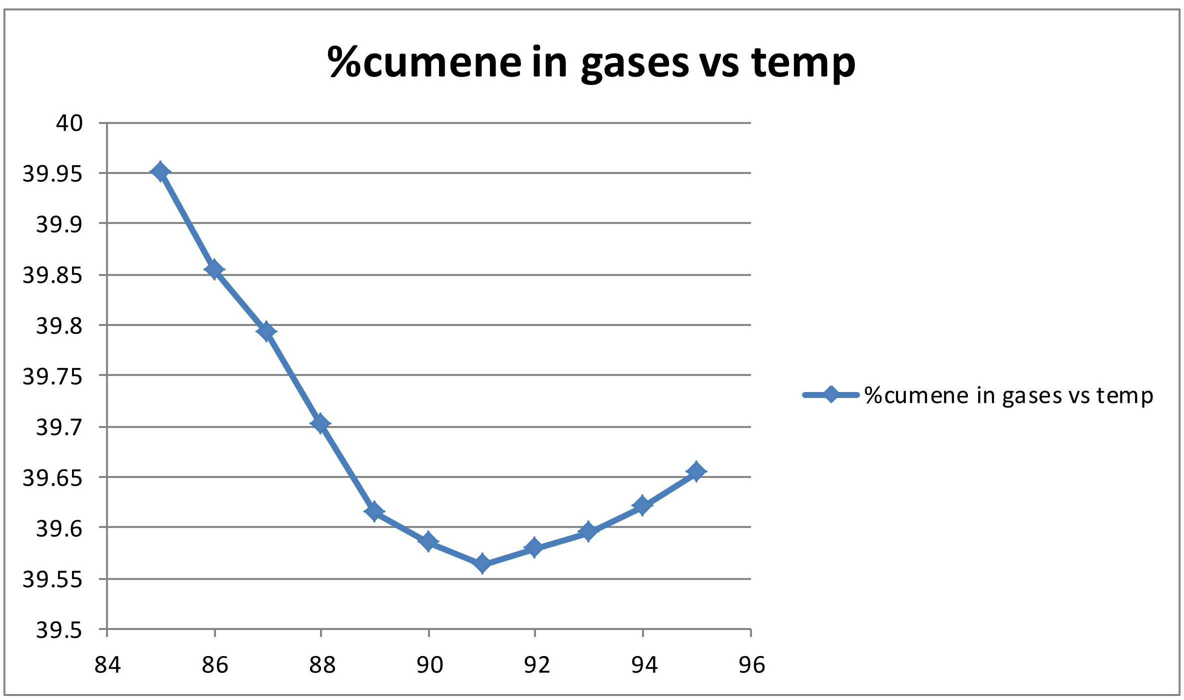


Figure 8: %Cumene in Gases Vs Flashing Temperature

From the above plots, it was observed that as the temperature is increased, the percentage of cumene in the product stream increased initially until a temperature of 91°C was reached and then a gradual decrease was observed. Similarly, with increase in temperature, the percentage of cumene in by-products and the vent gases decreased initially until a temperature reached around 91°C and then started increasing. According the above observation, it was found that the temperature of the flash tank cannot be kept neither very high nor very low.

Thus the optimum temperature of the flash tank was found out to be 91°C. Although there isn't a big variation in the flashing temperature from the Turton design, this small change could increase the efficiency by a small amount. The flow rate of the outlet stream at the optimized temperature was found out to be:

Table 7: Flow Rates of Products From Flash Tank

	Cumene (kgmol/hr)	Total Flow Rate (kgmol/hr)
Bottom Product	163.48	184.95
Gases	8.293	20.55

The bottom product from the flash tank acts as the feed to the benzene column where benzene and cumene are separated where benzene is recycled back to the feed and cumene is sent for further separation.

3.5 Benzene Column Design:

In the benzene column, the design specification is to separate the two components such that maximum amount of benzene should leave from the top as recycle benzene and cumene should leave as bottom product for further separation process. This ensures maximum purity in the cumene which is the main product in the process and also makes the process economical by recycling benzene to the feed stream of the reactor.

In the procedure followed for designing the benzene column, NRTL physical property package was used to make the calculations. The required data like temperature, pressure, number of stages, reflux ratio and feed tray location was taken from the Turton design and further optimization was done based on those values. The variables optimized in the process are reflux ratio, feed stage location and the number of stages. When one variable was being optimized, the other two were kept constant.

Reflux Ratio Optimization:

While the reflux ratio was being optimized, the number of stages was kept fixed and its value was taken to be 15 with reference to the Turton design. The reflux ratio was varied from 0.1 onwards and the percentage of cumene in the final product stream was considered to check for the best result. After the simulation was run, a graph was plotted between the two parameters which is shown below:

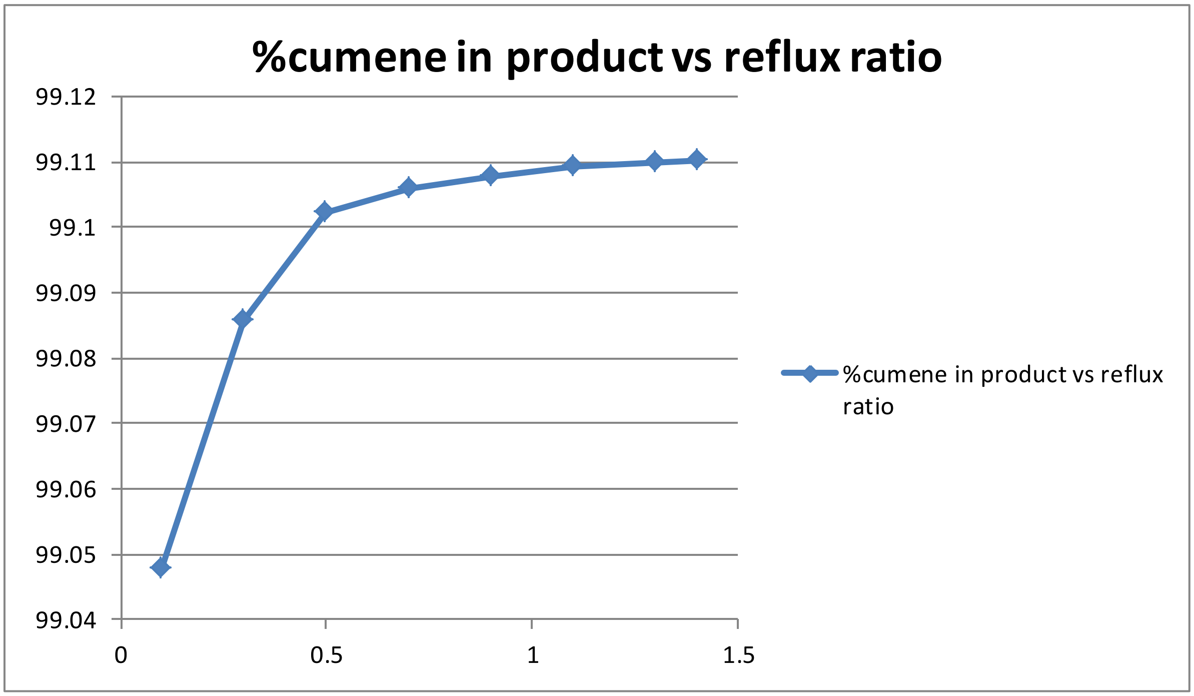


Figure 9: %Cumene in Product Vs Reflux Ratio

From the above graph, it was observed that as the value of reflux ratio was increased from 0.1 onwards, the percentage of cumene in product stream increased initially until a reflux ratio of 0.5 was reached and after that it becomes more or less constant. Even though a high value reflux ratio does ensure purity in the product but it leads to a higher reboiler heat duty which makes the process very uneconomical. So an optimum reflux ratio of 0.5 was chosen for the benzene distillation column.

3.5.2 Feed Tray Location Optimization:

The feed tray location is optimized by varying it and keeping the reflux ratio constant at 0.5 and number of trays at 15. The two parameters mainly affected due to the feed tray location and which decide the economic viability are amount of cumene in product stream and the reboiler heat duty. Therefore these variables are used to find the optimized result. Feed tray location was varied from 3 onwards and the graphs were plotted between the two parameters and the feed tray location and are shown below:

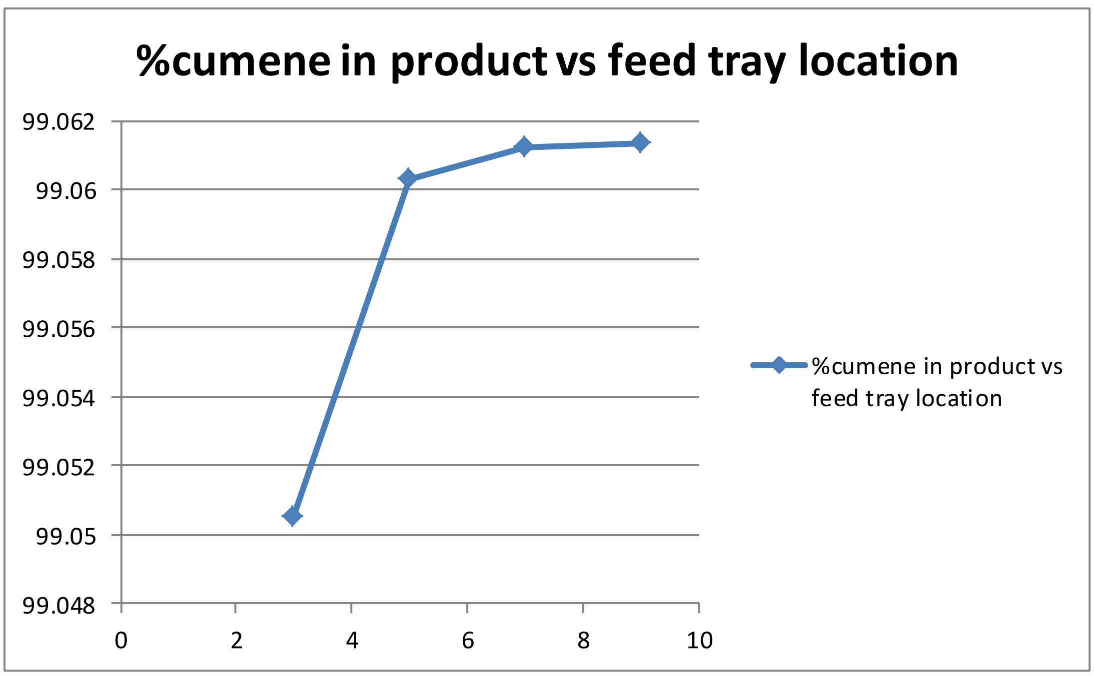


Figure 10: %Cumene in Product Vs Feed Tray Location

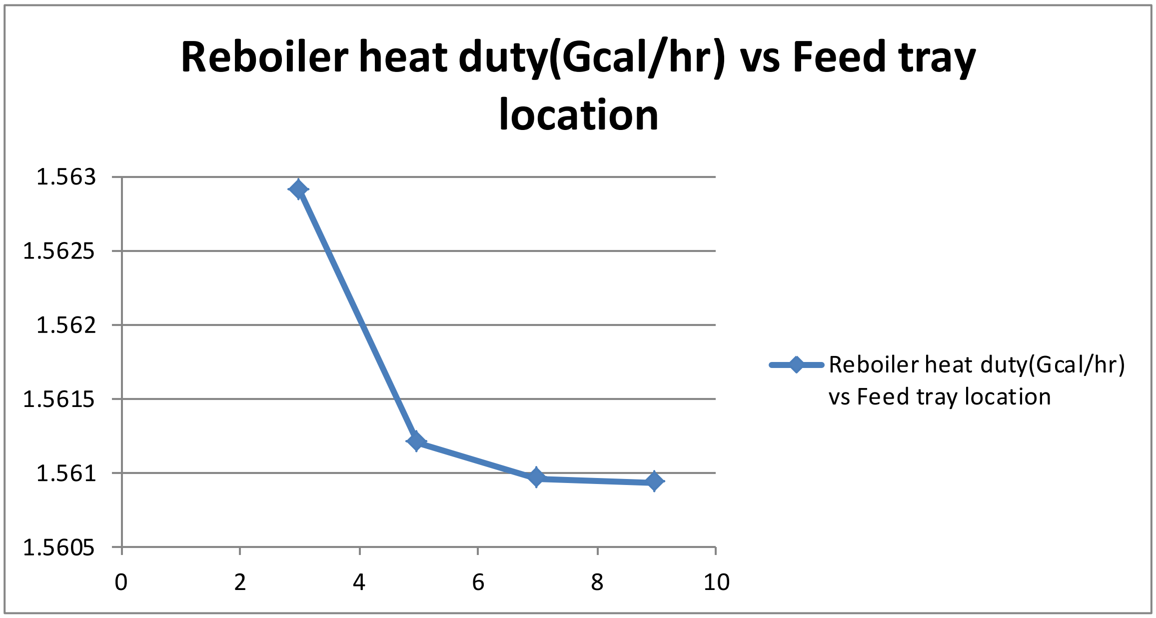


Figure 11: Reboiler Heat Duty Vs Feed Tray Location

From the above results, it was seen that the amount of cumene in the product stream increased rapidly in the beginning but as the feed tray location of 6 was reached, the graph became almost constant. Similarly, when reboiler heat duty was analyzed, the heat duty was very high initially. A high value of heat duty would have made the process very costly. As the feed tray location was increased, it was found that the heat duty reduced suddenly until a value of 6 to 8 was reached and then it became more or less constant. Therefore the optimized value of the feed tray location was taken to be 6 and was used to make the further calculations.

3.5.3 **Number of Trays Optimization:**

To optimize the number of trays, the amount of cumene in product and the reboiler heat duty were used again. The reflux ratio and the feed tray location were kept constant at their optimized value found previously. The number of trays was varied from 10 onwards and graphs between the two parameters and the number of trays to analyze the result. The graphs are as following:

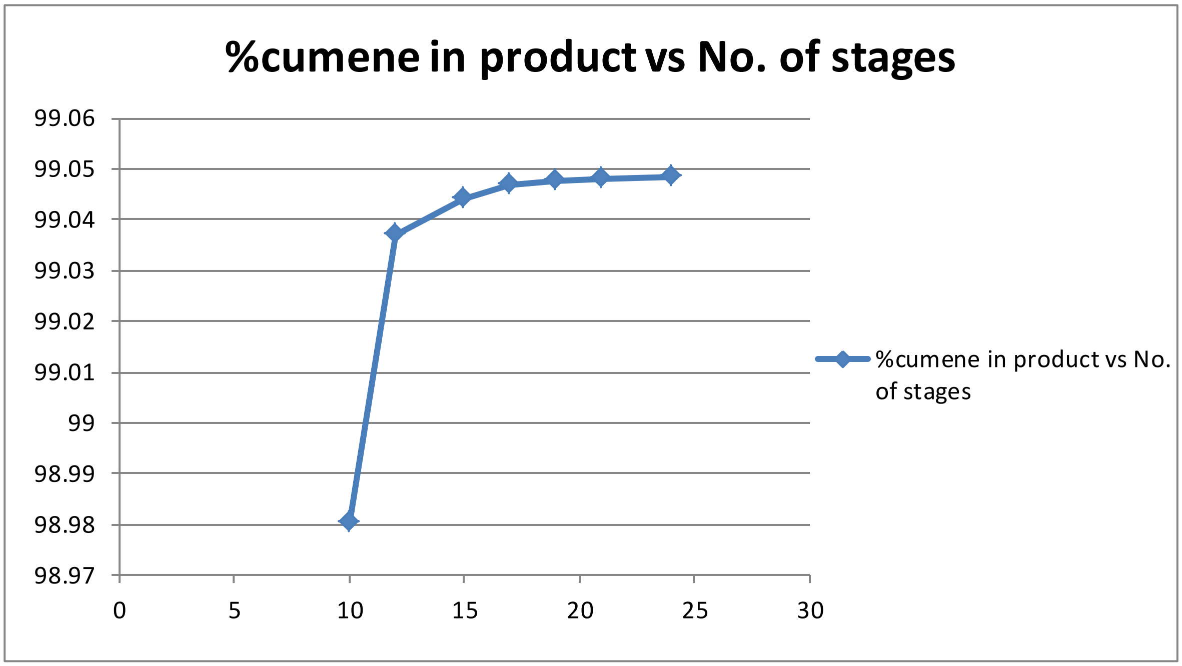


Figure 12:%Cumene in Product Vs No. Of Stages

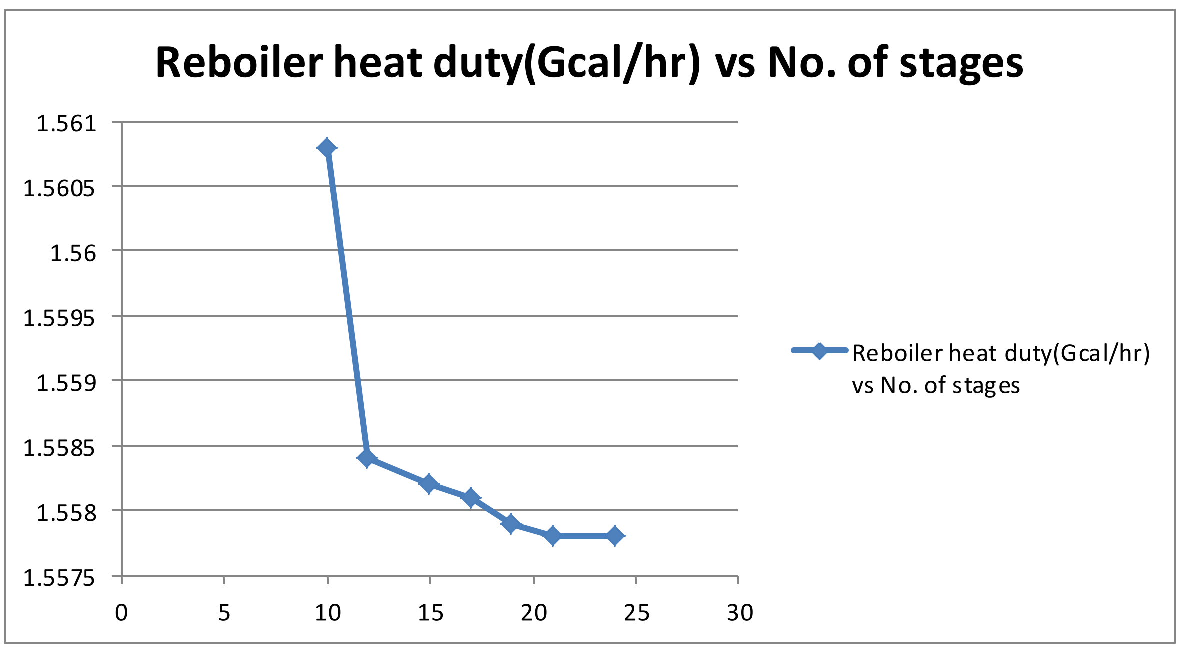


Figure 13: Reboiler Heat Duty Vs No. Of Stages

In this process also, the variation of amount of cumene in product was similar. As the number of trays was increased from 10 onwards, initially there was a steep rise in the graph. As the value of number of trays reached around 18, there was any considerable change above it. Similarly, when the number of stages was varied with reboiler heat duty, the heat duty decreased suddenly in the beginning. But after the value crossed 18, the change in the heat duty was negligible. Therefore, 18 was found as the optimum number of trays for the benzene column.

Finally, the optimized values for the benzene distillation column were as following:

TABLE 8: Optimized Results For Benzene Column

No. of Trays	18
Feed Tray Location	6
Reflux Ratio	0.5
Temperature	60°C
Pressure	1.75 bar

3.6 Cumene Distillation Column:

In the cumene distillation column, the design specification is to obtain maximum amount of cumene in the distillate and reduce its amount in the bottoms. The bottom product in this column contains mostly DIPB (di-isopropyl benzene) which is a by-product in the process. The optimization process is aimed at minimizing the production of the by-product and obtaining a balance between the amount of cumene and its purity.

In the procedure followed, NRTL physical property package was used again to make the calculations similar to benzene column. The properties optimized were reflux ratio, feed tray location and the number of stages. When one variable is being optimized, the other two are kept constant. As the process goes on, the optimized values are used instead of the basic values. The basic data like temperature, pressure etc was again referred from the Turton design and used in the simulation.

3.6.1 Reflux Ratio Optimization:

For the optimization process, the number of stages was kept at 20 with reference to the Turton design and the feed tray location was set at 12. The reflux ratio was then varied from 0.1 onwards. As the Txy diagram for the cumene-DIPB system was thinner than the benzene-cumene system, a comparatively higher value of reflux ratio is expected. For analyzing the results, amount of cumene in the product was chosen as the parameter. After obtaining the values of amount of cumene for different values of reflux ratios, they were plotted on a graph and further analyzed. The graph is shown below:

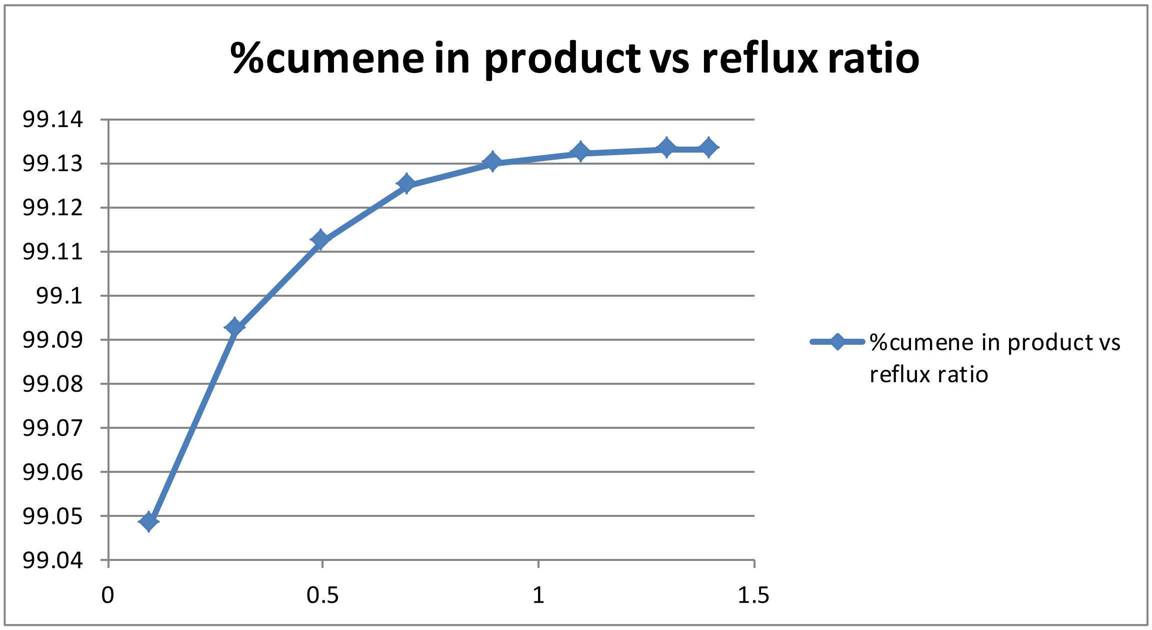


Figure 14: %Cumene in Product Vs Reflux Ratio

From the above graph, it can be seen that amount of cumene in product increases until a value of 0.6 is reached and then becomes more or less constant. As the reflux ratio cannot be increased beyond a certain limit because it may lead to increase in the reboiler heat duty which can make the whole process very uneconomical. Therefore, 0.6 is chosen as the optimum reflux ratio for the cumene distillation column.

3.6.2 Feed Tray Location Optimization:

In this process, similar to the benzene column, the reflux ratio is kept fixed at its optimized value i.e. 0.6 and the number of stages is taken as 20. Now to find out an optimized value, amount of cumene in product and the reboiler heat duty was chosen again. The feed tray location was varied from 7 onwards and the graph was plotted between the two parameters and the feed tray location. The graph is shown below:

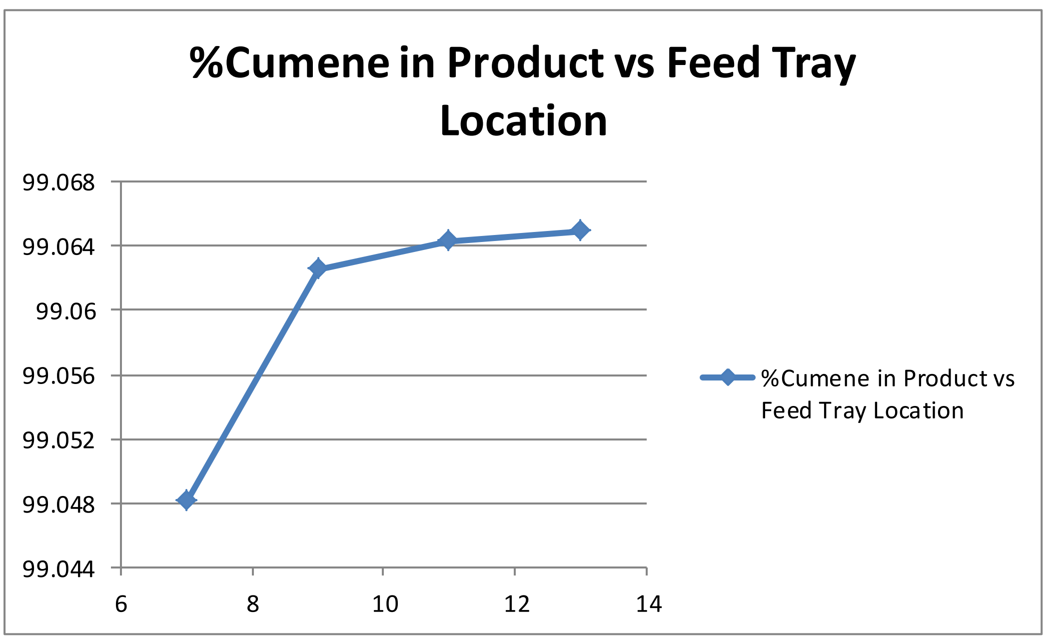


Figure 15: %Cumene in Product Vs Feed Tray Location

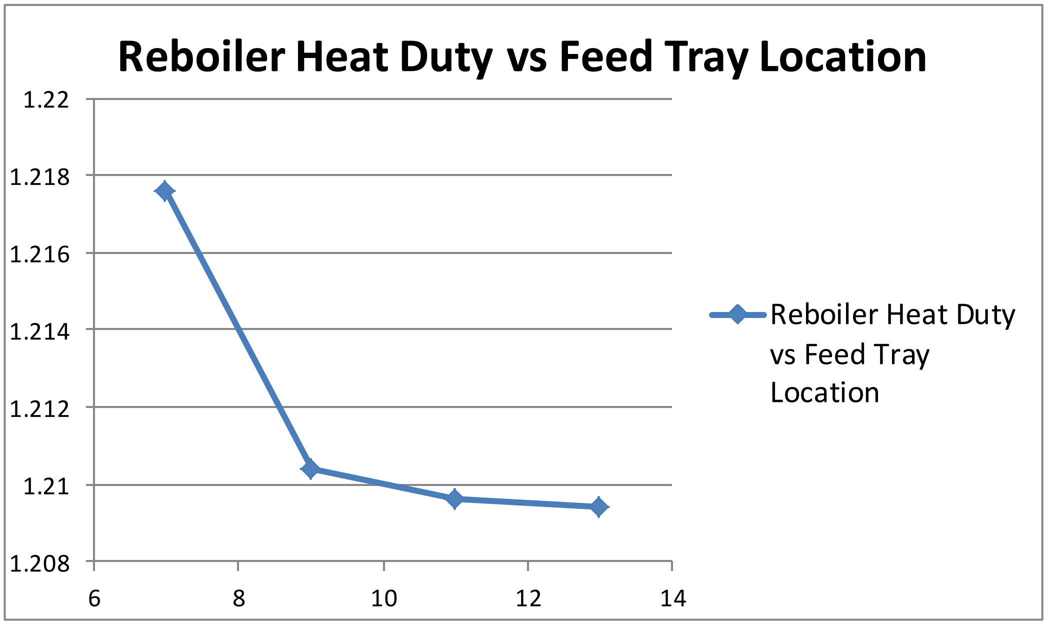


Figure 16: Reboiler Heat Duty Vs Feed Tray Location

It was seen that the graph followed the same patter as that for benzene column. According to both the graphs an optimum value of 11 was taken as the feed tray location. As the number of trays was kept at 20, a ratio of 2:1 was found out to be optimum for this column.

Number of Trays Optimization:

A similar process was followed for this optimization also. The reflux ratio was kept constant at 0.6 and the ratio of 2:1 was maintained to choose the feed tray location while varying the total number of trays. The variables used to optimize the number of trays were amount of cumene in product and the reboiler heat duty. The plots of these two parameters with total number of trays are shown below:

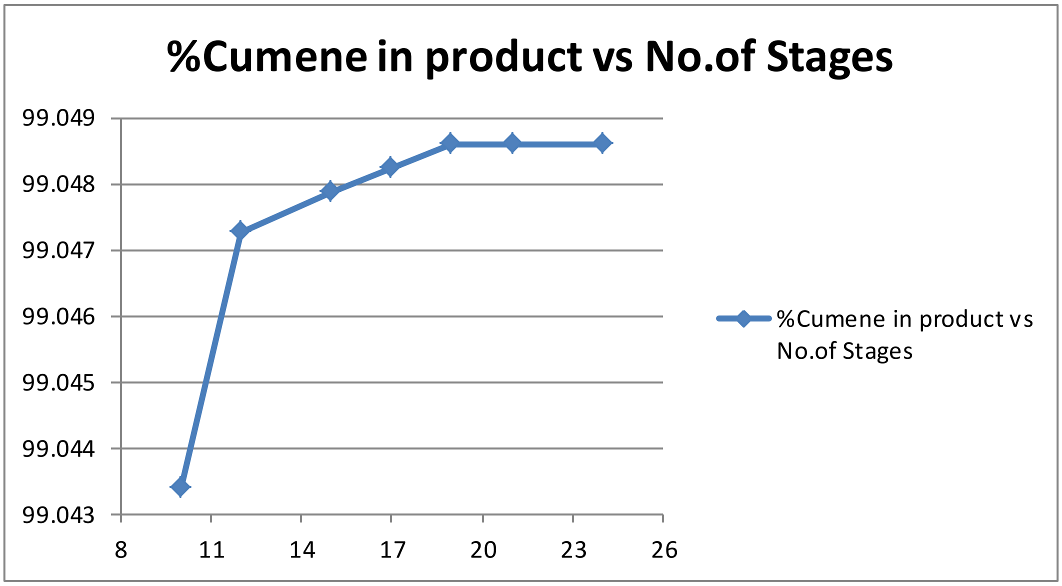


Figure 17: %Cumene in Product Vs No. Of Stages

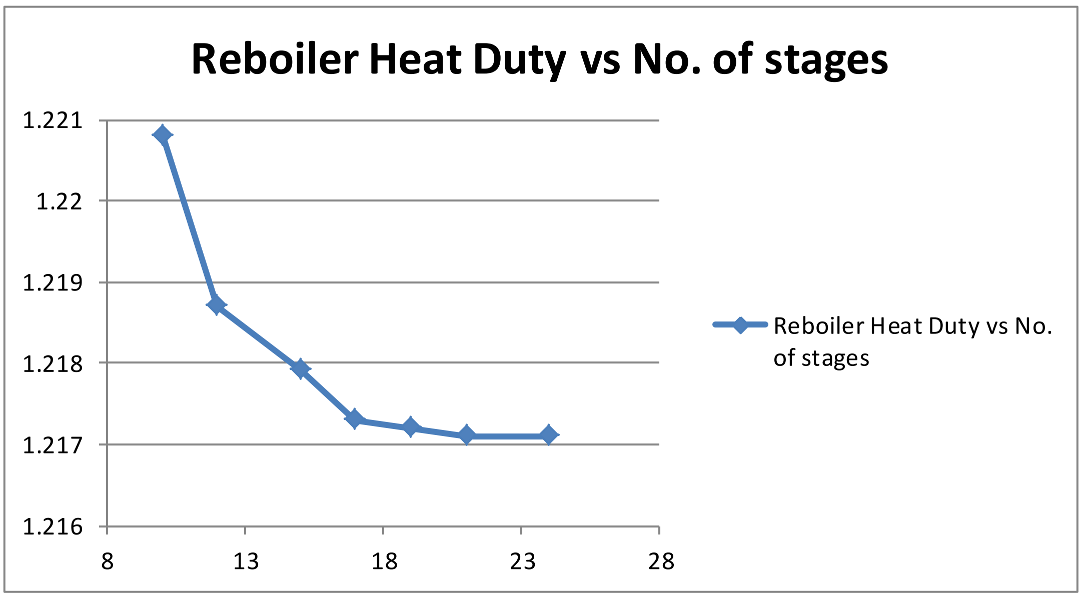


Figure 18: Reboiler Heat Duty Vs No. Of Stages

Again it was found out that there was a steep rise in the plot of amount of cumene initially upto a value of 19 but it became constant gradually. Similarly in the plot of reboiler heat duty, the heat duty was very high in the beginning. As the number of stages increased, the heat duty kept on decreasing until a value around 19 was reached. After this point the change became negligible. Therefore, an optimum value of 19 was chosen as the number of trays for the cumene distillation column.

Finally, the optimized values for the cumene distillation column are:

Table 5: Optimized Values for Cumene Column

Number of trays	19
Feed Tray Location	11
Reflux Ratio	0.6
Temperature	152°C
Pressure	1.75 bar

CHAPTER 4

CONCLUSIONS

4. CONCLUSIONS:

In the optimization process, main emphasis was given on saving the cost of raw materials rather than saving the energy and capital costs. The cumene process exhibits an interesting design feature in terms of the engineering trade-offs. The basic components of the cumene process are the reactor and the separator sections. Optimization in the reactor section was conducted and it was found that increase in the reactor size increases the cumene production and at the same time increases the capital investment. Therefore depending on the requirement of a particular industry it could be modified to provide the desired result. Since the cost of raw material is usually more than the cost of energy in any industry, this optimization could earn an industry appreciable amount of gain in the production.

Optimization of the reactor section was followed by the separation section. For checking the type of separation process required, VLE characteristics for the components were checked and it was found that the mixtures were non-azeotropic and easily separable. As flash distillation was done before fractional distillation, an optimum flashing temperature for the process was found out. The fractional distillation was carried out using two distillation columns namely, the Benzene column and the Cumene column. The parameters optimized in these columns were reflux ratio, feed tray location and number of trays in the column. Once the optimized values were found for one unit, they were utilized to carry out further calculations.

The design of this process is such that if costs like energy costs and capital investments are saved, then the cost of raw materials tend to increase and vice versa. Therefore, the industries have to strike a balance between the two according to their requirements. The main concern in this particular report was to save the cost of raw material due to its shortage and all the manipulations were carried out accordingly. This was based on the Douglas Doctrine which states that the costs of raw materials and products are usually much larger than the costs of energy or capital in a chemical process. Therefore the process must be designed (investing capital and paying for energy) so as to not waste feed stocks or lose products (particularly in the form of undesirable products). [Douglas, 1998]

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