Report of Cooperative Education

Study of Bypass Fresh Benzene Feed at Benzene Column in the Cumene Production Process

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A Report Submitted in Partial Fulfillment of the Requirements

for the Degree of Bachelor of Engineering (Petrochemical Engineering),

Department of Chemical Engineering, Faculty of Engineering,

King Mongkut's Institute of Technology Ladkrabang

Academic Year 2017

รายงานสหกิจศึกษาฉบับสมบูรณ์

การศึกษาการทำบายพลาสสายเบนซีนบริสุทธิ์ที่หอกลั่นเบนซีนในกระบวนการผลิตคิวมีน

นางสาวยสุตมา ดำรงมหาสวัสดิ์

รายงานนี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรวิศวกรรมศาสตรบัณฑิต

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สถาบันเทคโนโลยีพระจอมเกล้าเจ้าคุณทหารลาดกระบัง

ปีการศึกษา 2560

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ABSTRACT

Isopropylbenzene (cumene) is produced from the 2-step reaction process of benzene and propylene catalyzed by a regenerable zeolite-based catalyst. The primary alkylation reaction of benzene and propylene generates cumene, the intended product, and diisopropylbenzene (DIPB) as a by-product. Then, the DIPB is converted to cumene by reacting with benzene in the transalkylation reactor. The reactor effluents are fed into series of separation columns. Benzene column is used to separate benzene from cumene and heavier compounds. Regularly, fresh benzene enters the process at the top of this benzene column, to eliminate the contaminants; it is combined with the unreacted benzene, which together are recycled to the alkylation and transalkylation reactors. However, due to high purity of the fresh benzene, bypassing the fresh benzene from the column may decrease the energy consumption. In this work, Aspen Plus is used to help studying the effect of the bypassing. The results show that water concentration in benzene recycle stream after bypassing fresh benzene did not exceed the specification value even at the maximum bypass. Considering the minimum temperature of benzene recycle stream that was limited by alkylation reactor delta temperature due to its higher activity, the optimum percentage of bypassing is found to be 65%. Nevertheless, insignificant amount of energy consumption and cost were reduced. Moreover, the addition of the contaminants may lead to the increasing of the catalysts deactivation rates. Therefore, bypassing of the fresh benzene directly into the recycle benzene stream is not recommended.

Keywords: Simulation, Optimization, Benzene distillation column, Steam reduction, Cost saving

ACKNOWLEDGEMENTS

The success and the final outcome of this project required a lot of guidance and assistance from many people and I extremely provided to have got this all along the completion of my project. All that I have done is only due to such supervision and assistance and I would not forget to thank them.

I would like to make my deepest appreciation and gratitude to my mentor, Mr. Poochet Horkanya, process engineer at PTT phenol Co., Lltd for his valuable guidance, constructive criticism and encouragement during every stage of this project, without his which this project wouldn't have been possible.

I respect and thank my advisor, Dr. Wichitra Wongpromrat, for providing me an opportunity to do the cooperative with PTT phenol Co., Ltd and giving me all support and guidance which made me complete the project duly.

I heartily thank to my co-adviser, Dr. Amata Anantpinijwatna for his guidance and suggestions during this project work. Also, for teach me to use the AspenPlus.

I would not forget to thanks to PTT phenol Co., Ltd for kindness and taking care of me until the last day of cooperative. I'm very grateful.

I am thankful to and fortunate enough to get constant encouragement, support and guidance from all teachers of Chemical Engineering, King Mongkut's Institute of Technology Ladkrabang which help me to achieve the goal.

I really appreciate to my family for their support and always stay by my side.

Lastly, I would like to thanks myself for my patience, effort and optimist attitude that led me to overcome obstacles and problems.

Yasuthama Damrongmahasawat

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NOMENCLATURE

Name	Description
Components	
• Benzene [1]	Hydrocarbon compound with the chemical formula C_6H_6. It is toxic, volatile, flammable liquid hydrocarbon found in crude oil and as byproduct of oil-refinery process. Benzene is used as an industrial solvent as chemical intermediate and in paints, varnishes, etc. Benzene causes central nervous system damage acutely and bone marrow damage chronically and is carcinogenic. It was formerly used as parasiticide.
• Cumene [2]	Isopropylbenzene, commonly name is cumene. It is an aromatic hydrocarbon with the chemical formula C_9H_{12}, flammable colorless liquid. Cumene is the principal chemical used in the synthesis of industrially important chemical such as phenol and acetone. Minor uses of cumene include as a thinner for paint, constituent of some petroleum-based solvents, etc. Cumene may be moderately toxic by inhalation, ingestion and skin absorption.
• Diisopropylbenzene (DIPB) [3]	Cumene in the alkylation react with propylene and form DIPB. DIPB is a clear amber liquid with a sharp, penetrating odor. It has three isomers (ortho, meta, para). DIPB can be converted to cumene in transalkylation reaction.

CHAPTER I
INTRODUCTION

1.1 Company profile

PTT Phenol Co., Ltd. is an affiliation of the PTT Group. Its line of business is petro-chemical. Since 2013, PTT Phenol Co., Ltd. is wholly owned by PTT Global Chemical Co., Ltd. It has a 134-rai factory situated in the Hemarach Eastern or Map Ta Put, Muang Rayong District, Rayong Province. It manufactures phenol, acetone, and bisphenol A.

Currently there are two factories under PTT Phenol Co., Ltd. that comprise of:
1) Phenol factory manufactures 250,000 and 154,000 tonnes per year of phenol and acetone respectively;
2) Bisphenol A (BPA) factory has a manufacturing capacity of 150,000 tonnes per year.

PTT Phenol Co., Ltd is also considered the largest single unit or 'single train' in the world. The objective for establishment of this factory is to add value to the existing products since the condensation of phenol and acetone will yield BPA and polycarbonate (PC). PC is the high-value engineering plastic which can be used in automobile industry and the productions of medical equipment, computer and electronics' parts and component such as CDs and DVDs.

1.2 Involved process

The study process is the cumene production process. This process provides improvements compared to older cumene technology such as higher yield, lower investment and utility costs, reduction of solid waste, and better stability [4]. Raw materials, fresh benzene and propylene, are supplied by the PTT Global Chemical Co., Ltd. The focus unit in this work is the benzene distillation column that will be mentioned as benzene column in the following.

1.3 Background of the project

Benzene column is used to separate benzene from cumene and heavier compounds. Regularly, fresh benzene enters the process at the top of this benzene column, to eliminate the contaminants; it is combined with the unreacted benzene which together are recycled from the alkylation and transalkylation reactors. After fractionation both feeds, benzene is directed to the alkylation and transalkylation reactors for converting to cumene. High pressure steam is used at the reboiler of the column to boil up benzene and other compounds in the benzene column. However, due to high purity of the fresh benzene, bypassing the fresh benzene from the column may decrease the energy and high-pressure steam consumptions.

1.4 Objectives of the project

1.4.1 To evaluate amount of high pressure steam consumption at benzene column after bypassing fresh benzene.

1.4.2 To analyze the quality of distillated benzene recycled which includes benzene purity, water content and temperature of recycled stream as control specification.

1.4.3 To find the optimum condition to do the bypass.

1.4.4 To evaluate the feasibility and benefit of bypassing the fresh feed benzene through the benzene column.

1.5 Scopes of project

1.5.1 Energy consumption and distillation at benzene column in cumene production process of the PTT Phenol Co., Ltd. (designed by UOP) were considered.

1.5.2 This project used Aspen Plus program for evaluating and analysis.

CHAPTER II

LITERATURE REVIEW

2.1 Process description

Q-Max [5] is the process that converts benzene and propylene into high quality cumene (99.92 %wt) using a regenerable zeolite-based catalyst. A process flow diagram is shown in Figure 2.1. The process can be separated into 2 sections which are the reaction section and fractionation section. There are 2 reaction steps in the reaction section. The primary reaction is called alkylation where cumene (intended product) and DIPB (by-product) are produced from the reaction of benzene and propylene. The second reaction step is transalkylation where DIPB reacts with benzene to form the cumene.

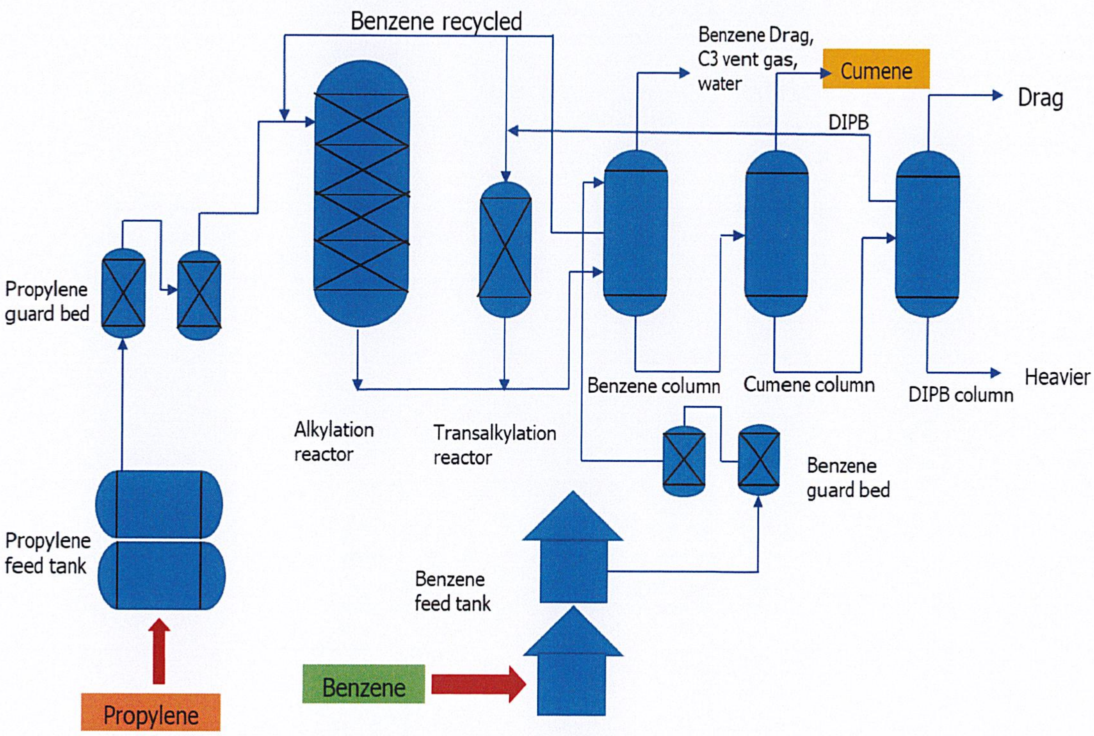


Figure 2.1 The process flow diagram.

As shown in the Figure 2.1, propylene from the propylene guard bed is directly fed to the alkylation reactor and is combined with the benzene from the benzene column to produce cumene.

An effluent from the alkylation reactor combined with the transalkylation reactor's effluent is fed to the benzene column to separate benzene, cumene and others (the major components are heavier compounds). Fresh benzene from benzene guard bed is sent to the top of the benzene column and is combined with unreacted benzene from mixed effluents of alkylation and transalkylation reactors. Then, overhead benzene from the benzene column is recycled to the alkylation and transalkylation sections. A small drag benzene stream is taken from the benzene column overhead to purge non-aromatics that concentrate in benzene stream. The product at the bottom of benzene column is fed to the cumene column where the main product, cumene, is separated from the heavier aromatics. The bottom of cumene column contains mostly DIPB which is then fed to the DIPB column to separate the DIPB from heavies. The DIPB is recycled to the transalkylation reactor for converting to cumene. The heavy stream from bottom of DIPB column contains heavy aromatics which is used as fuel or blended with another refinery product. The drag stream from the overhead of DIPB column can be taken to remove impurities that have boiling point between cumene and DIPB such as cymene and butylbenzene.

2.2 Process principles

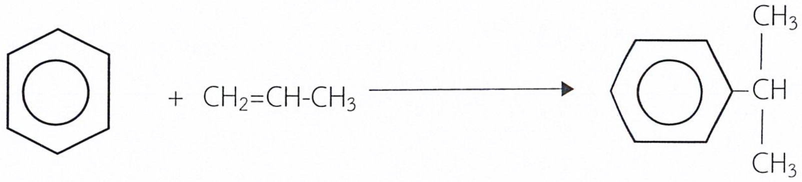
2.2.1 Catalyst

Alkylation and transalkylation reactions take place at the acid sites of the zeolite catalyst. The reactants diffuse through the catalyst pores to the active sites where they react. The reaction product diffuses through the catalyst pores back into the bulk process stream. The size of the pores limits the movement of large molecules resulting in improvement of selectivity compared to non-zeolitic catalysts [1].

2.2.2 Alkylation chemistry

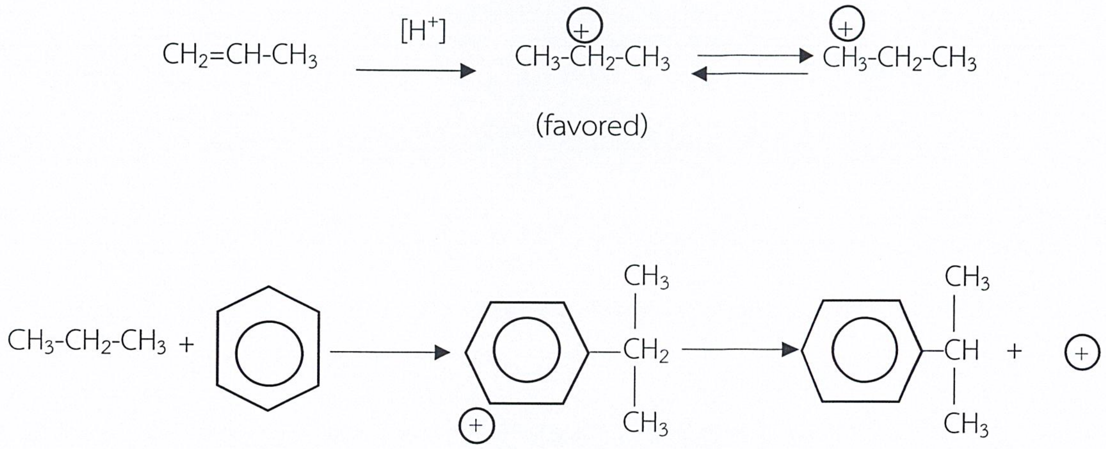
Benzene reacts with propylene in the alkylation reactor over zeolite catalyst to form cumene. The reaction is exothermic and the conversion of propylene is completely 100%. The heat of the reaction causes the increasing of temperature across the reactor. The acid function of the zeolite donates a proton to a propylene molecule to form a highly reactive carbonium ion. The carbonium ion then produces an electron bond with the benzene molecule releasing the proton for further reaction. Proton donors in decreasing strength are inorganic acids, Lewis acids, Bronsted acids, and zeolite catalysts.

Primary reaction



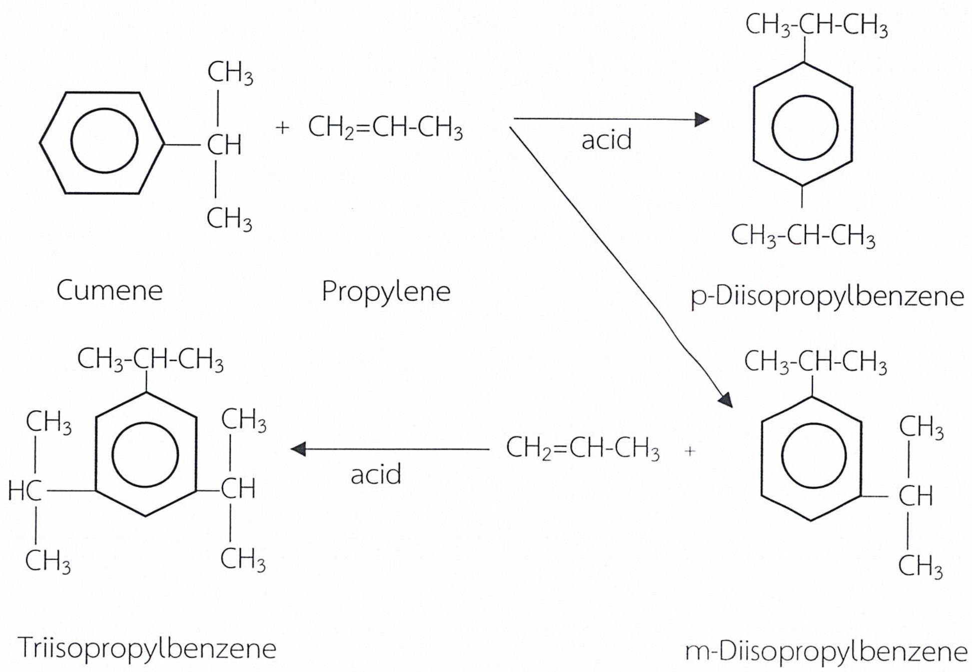
Benzene Propylene Cumene

Reaction mechanism



Another major alkylation reaction is cumene reacting further with propylene to form diisopropylbenzene (DIPB). There are 10-20% of DIPB found in the alkylation reaction products.

Secondary reaction

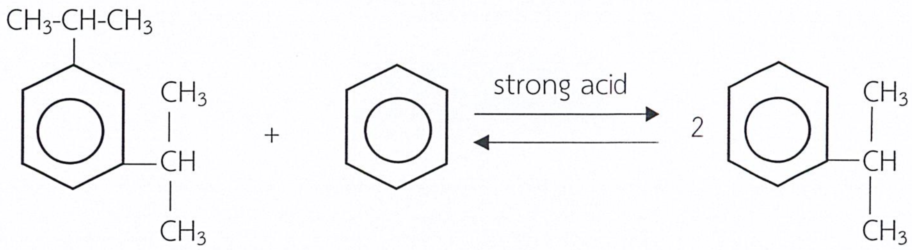


2.2.3 Transalkylation chemistry

In the transalkylation reactor DIPB produced from alkylation reaction is converted back to an equilibrium mixture with a higher concentration of cumene. For the reaction propyl groups are transferred from one phenyl ring to another. One benzene molecule reacts with one DIPB molecule to produce two molecules of cumene.

The reaction of DIPB and benzene to form cumene which is reversible reaction operates at a much slower rate than the reaction of benzene and propylene. For the given catalyst bed size, the conversion of DIPB to cumene is increased by a longer residence time, high benzene to DIPB ratio, and high reactor temperature.

Primary Reaction



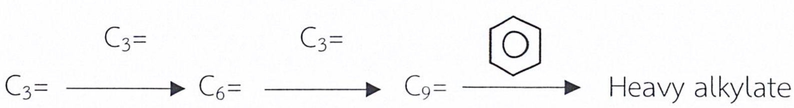
Diisopropylbenzene (DIPB) Benzene Cumene

2.2.4 Side reactions

Besides the alkylation reaction between benzene and propylene, all acid catalysts promote the following undesirable side reactions

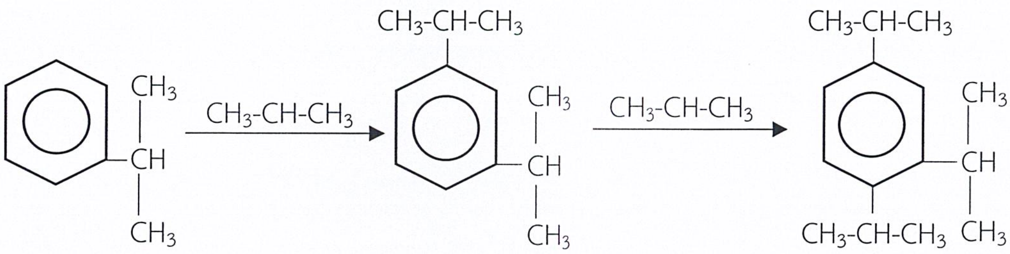
- *Oligomerization of olefins* [6]. The method for acid-catalyzed alkylation is the diffusion of olefin to an active site saturated with benzene and is then followed by adsorption and reaction. One possible side reaction is the combination of propyl carbonium ion with propylene to form a C_6 olefin or even further reaction to form C_9, C_{12} or heavier olefins.

Olefin Oligomerization



- *Alkylation of benzene with heavy olefins* [6]. Once heavy olefins have been formed through oligomerization, they may react with benzene to form hexylbenzene and heavier alkylated benzene by-products.
- *Polyalkylation* [6]. The addition of an isopropyl group to the benzene ring to produce cumene weakly activates the ring toward further substitution, primary at the meta and para position, to make DIPB and heavier alkylates.

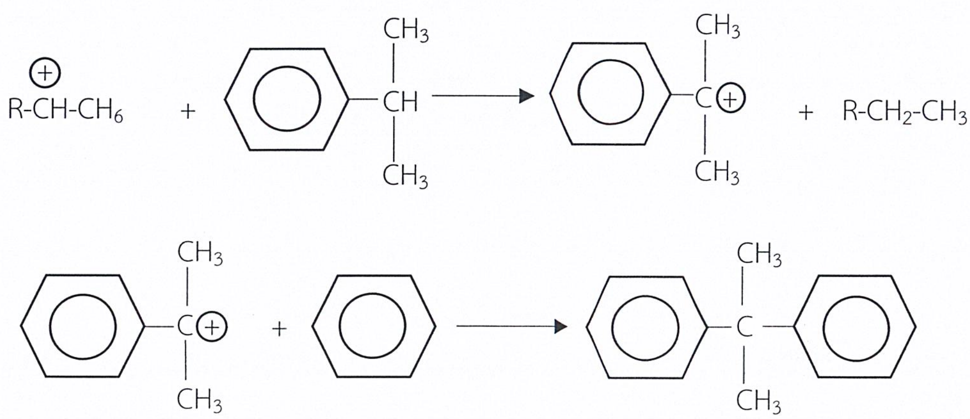
Polyalkylation



Cumene Diisopropylbenzene Triisopropylbenzene

- *Hydride-transfer reactions* [6]. Transfer of hydrogen to an olefin by the tertiary carbon on cumene can form a cumyl carbonium ion that may react with second benzene molecule to form diphenylpropane.

Hydride Transfer



Diphenylpropane

2.2.5 Feed contaminants

Impurities that enter the reactor either with the benzene or propylene may react to form the compounds leading to reduce the cumene yield. Some of common feed contaminants and their effects are as follows.

Ethylene

Ethylene in feed reacts with benzene to form ethylbenzene that is the cumene product impurity. The catalyst generates a very small amount of ethylbenzene from either olefin oligomerization if ethylene exists in the feed or cracking if there is no ethylene in feed. The cumene product typically contains 10-50 ppm ethylbenzene.

Toluene

Toluene can be present in benzene and reacts with propyl to form cymene. Cymene contaminating in the process can be removed from the DIPB column overhead.

n-propylbenzene

The n-propylbenzene(NPB) is produced from trace levels of cyclopropane in the propylene feed. Cyclopropane reacts with benzene to form either cumene or NPB.

2.2.6 Catalyst poisoning

Sulfur

Sulfur can be found in propylene or benzene feed and results in sulfur products. Sulfur in the propylene generally stays in the propane product while sulfur in the benzene tends to be cyclical in nature or sulfolane. Sulfur compounds such as thiophene are slightly basic and thus act as a temporary catalyst poison. Large quantities of sulfur in the propylene feed also suppress catalyst activity, decrease in yield and increase in impurities in cumene product such as olefin.

Nitrogen

Nitrogen is a catalyst poison. Common example of basic nitrogen compounds is amine. Amine are in the pretreatment units. It typically removes sulfur from the propylene feed. Basic nitrogen compound neutralizes acid sites on the catalyst and can only be removed from the catalyst by performing a carbon burn regeneration.

Oxygen

Oxygen can enter the unit in several ways such as a vacuum leak, use of aerated water in the propylene pretreatment section, and absorption of air in the benzene feed tanks. Oxygen can be stripped from benzene with water, such as in the benzene column. Oxygen reacts with cumene to form the hydroperoxide. Cumene hydroperoxide reacts in the unit to form phenol and acetone. Oxygen contamination generally results in high level of phenol in cumene product.

2.3 Process variables

Process variables are the parameters used to optimize the operation of cumene production process and to evaluate unit performance.

2.3.1 Independent variable

2.3.1.1 Alkylation reactor section

Benzene/Propylene ratio

Benzene/Propylene ratio is the main performance variables in the alkylation reactors. The B/P ratio has a direct impact on the catalyst stability and cumene yield with the order catalysts. If the ratio goes below design, more DIPB and heavier compounds are formed and the selectivity to cumene will be dropped while the most recent catalyst stability is not affected.

Bed inlet temperature (s)

The temperature in catalyst bed affects the stability of the catalyst, the reaction rate, and NPB formed in the alkylation reactor. The bed inlet temperature is normally 138 to 165°C. At high temperature, catalyst stability is better but NPB production is increased (decrease in cumene selectivity).

Bed Delta T (s)

The maximum target delta T's must not be higher than 14°C for maintaining high rate of alkylation reaction. A higher delta T than design results in more NPB formation due to the maximum temperature in the bed. Bed outlet temperatures and delta T's should be regularly monitored.

Liquid Hourly Space Velocity (based on Propylene)

Liquid Hourly Space Velocity (LHSV) based on propylene can be defined as volumetric flow of propylene through the reactor/catalyst volume. If the space velocity is low (flow through the reactor is low), there is an increase in the number of side reactions, resulting in a decreased selectivity. The higher NPB content is formed when LHSV is decreased at a given temperature.

Effluent recycle flow rate

The purpose of the effluent recycle is to minimize the temperature rising across the alkylation reactor (delta T control). The increase in temperature should be maintained less than design to maximize catalyst stability and minimize NPB formation.

Reactor pressure

The pressure is set to make the components being in liquid phase plus some margin. With the reaction components in the liquid phase, the change in pressure has no effect on the process.

Water content

No free water should be sent to the reactor under normal operating conditions. As water increase, the alkylation selectivity decreases and the reactor inlet temperature should be increased.

Feed properties

Impurities in either the propylene or benzene feed reduce the product yield. The change in the propylene content in the propylene feed directly affects the amount and quality of the cumene produced.

2.3.1.2 Transalkylation reactor section

Phenyl/Propyl ratio

Phenyl/Propyl ratio can be defined as moles of benzene (phenyl) groups/moles of propylene (propyl) groups. Each molecule of benzene has 0 propyl and 1 phenyl group. Each molecule of DIPB has 2 propyl groups and 1 phenyl group. Each molecule of cumene has 1 propyl and 1 phenyl groups. If the P/P ratio is too low (benzene flow is reduced or the DIPB flow is too high), DIPB conversion will decrease and heavies formation will increase.

Inlet temperature

As the transalkylation catalyst ages, it is necessary to increase the temperature to maintain the same conversion of DIPB to cumene. If the temperature is set too high, conversion will also increase but the selectivity will decrease. NPB production from the transalkylation reactor will also increase with increasing temperature.

Reactor pressure

As with the alkylation reactors, the pressure is kept high enough to keep all components in the liquid phase. The pressure is kept at the design value during normal operation.

Water content

Feed to the transalkylation reactor should be free water. An increase in water to the reactor decreases catalyst activity. Water desorbs from the catalyst and the temperatures are reduced, so higher reactor temperatures are required to compensate. The transalkylation reaction is much more sensitive to water than the alkylation reaction.

Feed properties

Heavies in the feed to the transalkylation reactor reduce conversion and deactivate catalyst.

2.3.1.3 Catalyst quantity

Amount of catalyst loaded into the reactor is usually fixed and is not changed during normal operation. Sometimes extra catalyst is added to the last bed (bottom) to maintain 100% conversion during plant upset. The catalyst quantities can change based on the improvement of feedstocks and revamps to unit capacity.

2.3.1.4 Fractionation section

Reflux ratio

Reflux ratio is used to control column operation in the fractionation section. Increasing reflux ratio will increase the purity of the top and bottom cuts. However, there is a limiting point. Above the certain level, there is the risk of liquid flooding internally in the column. The optimum ratio must be kept to provide an acceptable purity of the product and minimizes the utility cost of the column.

Heat Input

The heat input in the column is related to the reflux ratio.

Compositional Control

Compositions are maintained by controlling the temperature of each tray in the column that can be adjusted by either reflux or other major variables.

2.3.2 Dependent Variables

2.3.2.1 Alkylation reactor section

Propylene conversion

Propylene conversion is always 100% because excess benzene is fed to the reactor.

Mono-alkylation yield

The mono-alkylation yield is defined as the percentage of cumene formed in the alkylation section relative to cumene, DIPB, and heavies. This yield is affected by benzene/propylene ratio, LHSV, reactor temperatures and catalyst types.

n-propylbenzene (NPB) by-product formation

The amount NPB in the alkylation reactor is affected mainly by reactor temperatures and the amount of cyclopropane in the propylene feed. The tendency of NPB formation decreases with lowering the reaction temperature.

Catalyst activity & stability

The activity and stability are determined by carefully monitoring the temperature profile in the alkylation catalyst bed. The main variables affecting alkylation catalyst activity and stability are benzene/propylene ratio, space velocity, and catalyst temperature.

2.3.2.2 Transalkylation reactor section

DIPB conversion (Transalkylation reactor)

DIPB conversion is used to monitor the overall total reaction of DIPB in the transalkylation reactor.

Liquid Hourly Space Velocity (based on DIPB)

As DIPB increased, LHSV must be higher to maintain the same DIPB conversion, however, NPB formation is also higher. The LHSV of DIPB is set based on the amount of DIPB leaving the alkylation section and the temperature of transalkylation and phenyl/propyl ratio in the transalkylation reactor.

n-propylbenzene formation

The amount of NPB in the transalkylation reactor is affected mainly by DIPB conversion and reactor temperatures. Also, the NPB produced in the alkylation reactor influence the production of NPB in transalkylation reactor.

Catalyst activity and stability

The main variables that affect catalyst activity and stability are LHSV, reactor temperature, phenyl/propyl ratio, and water contents.

2.3.2.3 Overall Plant

Product quality

Quality of the cumene product depends on the amount of impurities in the stream. The product quality is dependent on feedstock impurities, the operating condition of the fractionation section and also the good circumstances of fractionation column internals, such as distributors, packing and trays.

Cumene yield

Cumene yield is affected by reactor conditions and fractionation conditions. The yield is generally greater than 99%.

2.4 Benzene column

The main feed to benzene column is fresh benzene from the benzene guard bed and the effluents from alkylation and transalkylation reactors. Benzene column has 60 trays. The number of trays affects the amount of reflux. The column is reboiled with high pressure steam (40 bar) to separate benzene from cumene and other compounds.

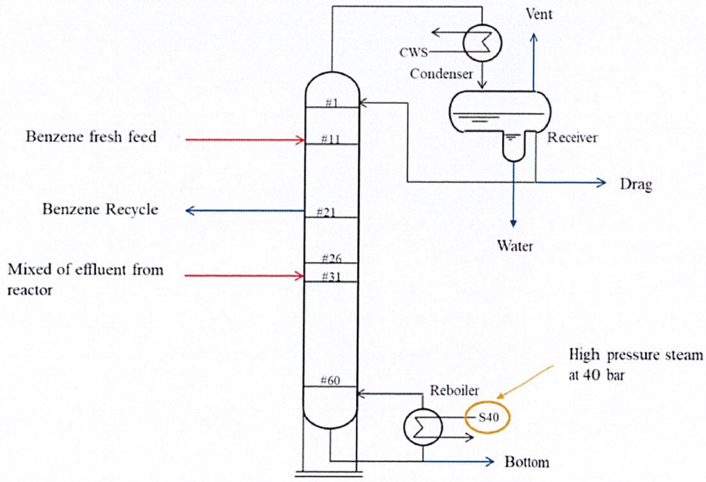


Figure 2.2 Benzene column.

Fresh benzene is brought into the top of the benzene column at 11th tray to strip out the water and oxygen from the fresh benzene. The mixed of alkylation and transalkylation reactor effluents enters at 31st tray of the column. The components in the vapor phase at top of the column are condensed in a benzene column condenser and are collected in a receiver. A benzene drag stream is sent to the overhead of the receiver to control the quantity of non-aromatics in the benzene stream. Benzene recycled stream is taken off the side-cut of the column at 21st tray to alkylation and transalkylation reactors. Recycled benzene is taken to maintain at least 90% of purity in benzene recycled stream for sending to the alkylation and transalkylation processes. The lower purity of benzene recycled stream than 90% is not practical because it requires higher utilities to maintain a constant benzene/propylene ratio in alkylation and phenyl/propyl ratio in transalkylation. The product stream at the bottom of benzene column is then sent to the cumene column to separate cumene and heavier compounds. The main idea for this column is to keep the minimum benzene in the cumene bottoms.

CHAPTER III

RESEARCH METHODOLOGY

3.1 Design procedure

The study procedures are presented in Figure 3.1.

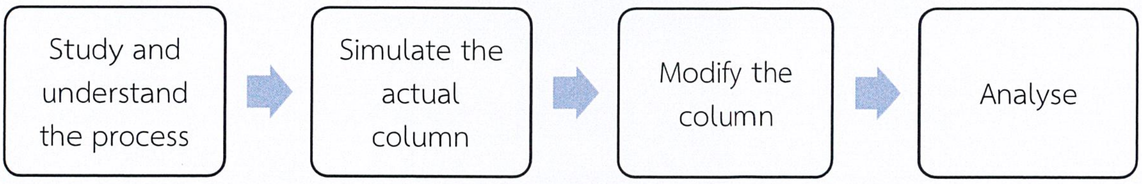


Figure 3.1 The study procedures.

3.1.1 Study and understand the process

The overall process is reported in Chapter 2.

3.1.2 Simulate the actual column

- List all involved components, model and equipment.
- Simulate the process.
- Control benzene quality with APEN's Design-Spec.

Table 3.1 Component lists of actual column.

No.	Name	Formula	Molecular weight	Boiling point (°C)
1	Water	H_2O	18.02	100
2	Propane	C_3H_8	44.1	-42.04
3	Butane	C_4H_{10}	58.12	-0.5
4	Benzene	C_6H_6	78.11	80.09
5	Hexane	C_6H_{14}	86.18	68.73
6	Toluene	C_7H_8	92.14	110.63
7	Heptane	C_7H_{16}	100.2	98.43
8	Ethylbenzene	C_8H_{10}	106.17	136.2
9	Cumene	C_9H_{12}	120.19	152.41
10	n-propylbenzene	C_9H_{12}	120.19	159.24
11	tert-butylbenzene	$C_{10}H_{14}$	134.22	169.15
12	sec-butylbenzene	$C_{10}H_{14}$	134.22	173.33
13	p-cymene	$C_{10}H_{14}$	134.22	177.13
14	p-DIPB	$C_{12}H_{18}$	162.27	210.5
15	TIPB	$C_{15}H_{24}$	204.35	238
16	2,2DPP	$C_{15}H_{16}$	196.29	281.19

Radfrac is selected for designing the benzene column. Soave-Redlich-Kwong equation of state (SRK) method has been selected as the thermodynamic model of this process. This unit is calculated by using standard convergence method and vapor-liquid as a valid phase. The pressure of the column is set to be 0.518 kg/cm^2 (g) for the condenser, 0.95 kg/cm^2(g) for the 1st stage of the column and the column pressure drop is 0.15 kg/cm^2 (g). The condenser temperature is kept constant at 34°C

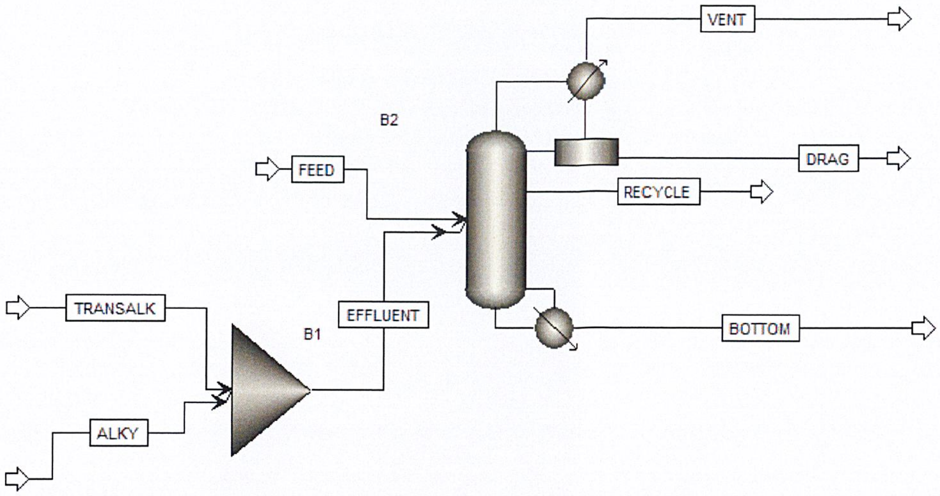


Figure 3.2 Flowsheet of actual column.

There are 62 trays in the column including condenser and reboiler with 2 inlet streams *(FEED, EFFLUENT)* and 4 outlet streams *(VENT, DRAG, RECYCLE, BOTTOM),* as shown in Figure 3.2, that are

- *FEED* refers to fresh benzene,
- *EFFLUENT* refers to the mixed of effluent streams from alkylation and trans alkylation reactors,
- *VENT* refers to C3 and C4 compounds in vapor phase,
- *DRAG* refers to non-aromatic compounds,
- *RECYCLE* refers to distillated benzene that will be sent to the reactors after fractionation.
- *BOTTOM* refers to cumene and heavier compounds.

The inlet stream conditions are showed in the Table 3.2. Fresh Benzene is fed at the 12^{th} tray and the mixed reactor effluent stream is fed at the 32^{nd} tray. Recycled stream is taken out at the 22^{nd} tray. Condenser type is partial-vapor-liquid and reboiler is kettle type. Distillate flow is fixed at 150 kg/h.

Table 3.2 Condition of inlet stream of actual column.

	Fresh benzene stream	Alkylation effluent stream	Transalkylation effluent stream
Temperature (°C)	32.7	162.8	126
Pressure ($kg/cm^2(g)$)	11	16.9	11.5
Mass flow (kg/h)	25275	57425	29472
Mass fraction			
Water	$1.12x10^{-04}$	$8.77x10^{-05}$	$1.64x10^{-04}$
Propane	0	$5.39x10^{-04}$	0
Butane		$1.41x10^{-06}$	$2.71x10^{-06}$
Benzene	0.9998	0.4236	0.5447
Hexane	0	$1.06x10^{-03}$	0
Toluene	$8x10^{-05}$	$1.06x10^{-04}$	$1.39x10^{-04}$
Heptane	0	$2.31x10^{-03}$	0
Ethylbenzene	0	$1.05x10^{-05}$	$3.26x10^{-04}$
Cumene	0	$4.92x10^{-01}$	$3.13\text{-}x10^{-01}$
NPB	0	$8.71x10^{-05}$	$9.32x10^{-05}$
TBB	0	$9.28x10^{-06}$	$4.77x10^{-06}$
SBB	0	$5.65x10^{-06}$	$3.69x10^{-05}$
p-Cymene	0	$3.21x10^{-05}$	0
p-DIPB	0	0.079	0.1336
TIPB	0	$5.38x10^{-04}$	$7.45x10^{-03}$
2,2DPP	0	$3.17x10^{-04}$	$7.84x10^{-04}$

The mass fraction of benzene in *BOTTOM* stream and the mass fraction of benzene in the *RECYCLE* stream are set by the *Design-Spec.* The mass fraction of benzene in *BOTTOM* stream is controlled by *RECYCLE* mass flow rate and mass fraction of benzene in the *RECYCLE* stream is controlled by the reflux rate of the column.

3.1.3 Modify the column

From the flowsheet (Figure 3.2), the splitter (*B3*) is added to separate *FEED* into *FEED2* and *BYPASS.* The mixer (*B4*) is added to mix the *BYPASS* and *RECYCLE* to be *RECYCLE2* stream as shown in the Figure 3.3. Then, the benzene bypass percentage is increased from 0 to 100% with a 5% interval.

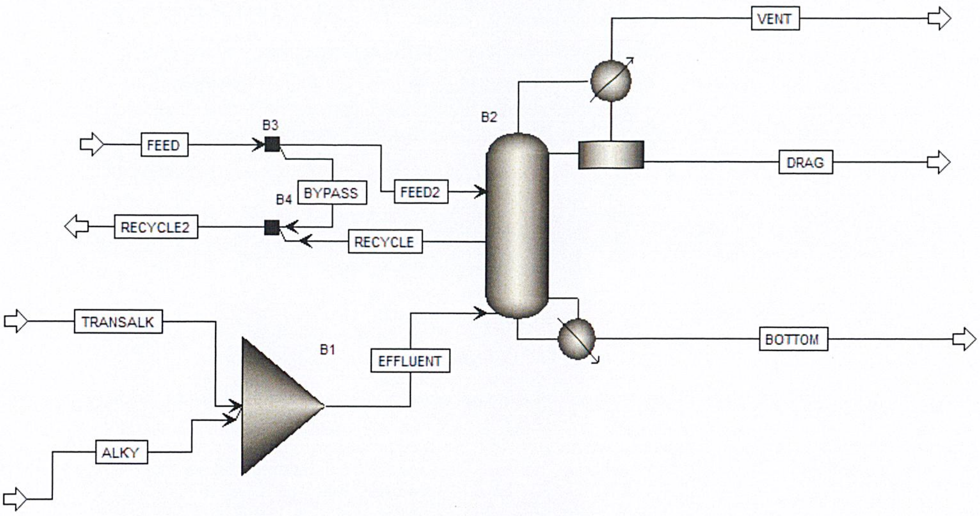


Figure 3.3 Flowsheet after modifying the column.

The mass fraction of benzene in *BOTTOM* stream and the mass fraction of benzene in the *RECYCLE2* stream are set by *Design Spec*. The mass fraction of benzene in the *RECYCLE2* and *BOTTOM* streams are controlled by varying the reflux rate of column and the *RECYCLE* mass flow rate respectively as shown in Table 3.3.

Table 3.3 Controlling benzene quality with the *Design Spec*.

Spec	Target	Vary	Upper	Lower
Mass fraction of benzene in *RECYCLE2* stream	0.9316	Reflux mass flow rate	20000	60000
Mass fraction of benzene in *BOTTOM* stream	$3.01\text{x}10^{-05}$	*RECYCLE* mass flow rate	35000	75000

CHAPTER IV

RESULTS AND DISCUSSION

4.1 Simulation results

Table 4.1 shows the results of simulation after bypassing the fresh benzene feed. Only 14 points from 21 points can be converged with the desired spec which are 0, 5, 10, 15, 20, 25, 30, 35, 45, 50, 55, 65, 70 and 75%. For the bypassing percentages more than 75%, the mass conservation of the column fails to do the bypass at specific *Deign Spec*.

Table 4.1 Benzene spec in *RECYCLE2* flow and *BOTTOM* flow in the different percentage of bypassing.

Bypass (%)	Mass fraction of benzene in *RECYCLE2* flow	Mass fraction of benzene in *BOTTOM* flow
0	0.9316	3.01×10^{-05}
5	0.9316	3.01×10^{-05}
10	0.9316	3.01×10^{-05}
15	0.9316	3.01×10^{-05}
20	0.9316	3.01×10^{-05}
25	0.9316	3.01×10^{-05}
30	0.9316	3.01×10^{-05}
35	0.9316	3.01×10^{-05}
40	0.761	0.0315
45	0.9316	3.01×10^{-05}
50	0.9316	3.01×10^{-05}
55	0.9316	3.01×10^{-05}
60	0.8077	0.0005
65	0.9316	3.01×10^{-05}
70	0.9316	3.01×10^{-05}
75	0.9316	3.01×10^{-05}
80	0.9314	0.0322
85	0.8667	0.1083
90	0.7904	0.0439
95	0.9435	0.0867
100	0.954	0.1018

At 40% of bypassing, material and energy balances fail to converge. The results in Figure 4.1 shown that the stage 22 (22^{nd} tray) is dried up and heat duty of reboiler is negative.

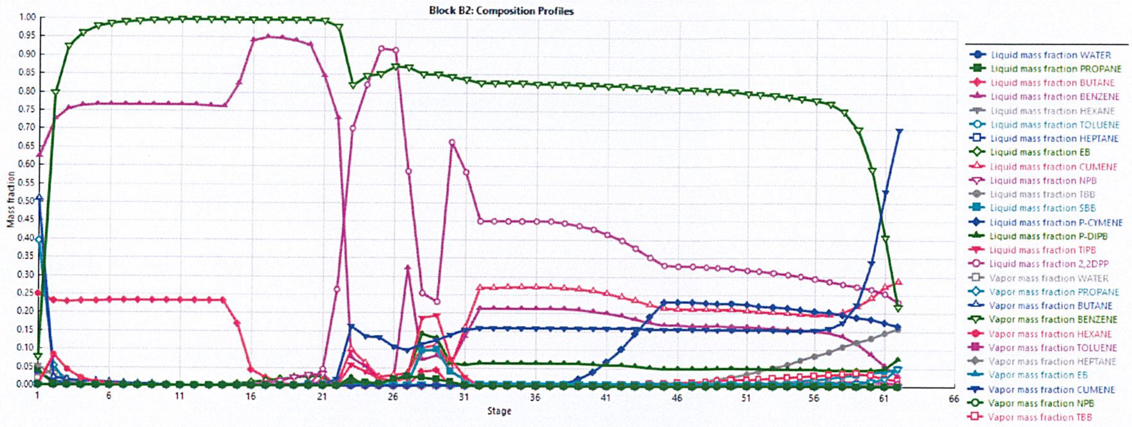


Figure 4.1 Composition profile at 40% of bypassing fresh benzene feed.

At 60% of bypassing, material and energy balances fail to converge. The results in Figure 4.2 show that the stages 22 (22^{nd} tray) and 31 (31^{st} tray) are dried up. Also, heat duty of reboiler is negative.

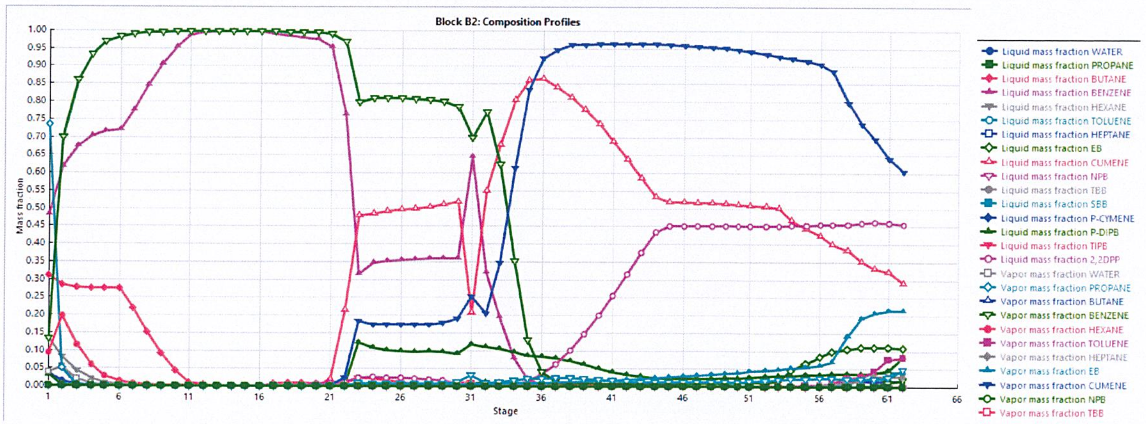


Figure 4.2 Composition profile at 60% of bypassing fresh benzene feed.

The error in the 40% and 60% of bypass may be caused by the fugacity calculations of the selected SRK equation of state. The equilibrium is calculated based on the fugacities of the liquid and vapor phases which are equal in this process. Thus, the equilibrium is failed leading to the mass balance error in the column calculation.

4.2 Simulation verification

Tables 4.2 and Table 4.3 show the condition accuracy in %error of the model comparing with the actual laboratory data. There is small difference in %error of considered variables obtained from the simulation and laboratory data (all data are reported in Appendix A1), so this model is verified.

Table 4.2 Condition accuracy.

	% Error	
	RECYCLE stream	*BOTTOM* stream
Temperature	0.45	0.81
Pressure	0	0
Mass flow	2.42	2.75

Table 4.3 Mass fraction accuracy.

	% Error	
	RECYCLE stream	*BOTTOM* stream
Water	13.6	N/A
Propane	21.2	N/A
Butane	N/A	N/A
Benzene	1.4×10^{-05}	0.07
Hexane	53.3	N/A
Toluene	37.8	572
Heptane	71.7	172
Ethylbenzene	75.2	86.3
Cumene	9.61	1.93
NPB	77.3	9.37
TBB	N/A	7.08
SBB	N/A	4.38
p-Cymene	N/A	18.7
p-DIPB	99.7	4.21
TIPB	N/A	N/A
2,2DPP	N/A	N/A

4.3 Effect of bypassing

4.3.1 Effect of bypassing on the utility and reflux

Increased in percentage of bypassing causes lowering the amount of benzene fractionated and helps to reduce the consumption of high pressure steam at the reboiler as shown in the Figure 4.3 (more details are reported in Appendix A2). It can be seen that, at the maximum bypass (75%), only 3.26 kg/h of high pressure steam is reduced. However, there are 2 inlet streams fed to the column that are fresh benzene stream (*FEED*) and the mixed of effluents from alkylation and transalkylation reactors (*EFFLUENT*). *EFFLUENT* flow rate remains unchanged, so the energy required for fractionating benzene from other components is almost the same. Therefore, the amount of high pressure steam used after bypassing is insignificantly decreased as shown in Figure 4.3

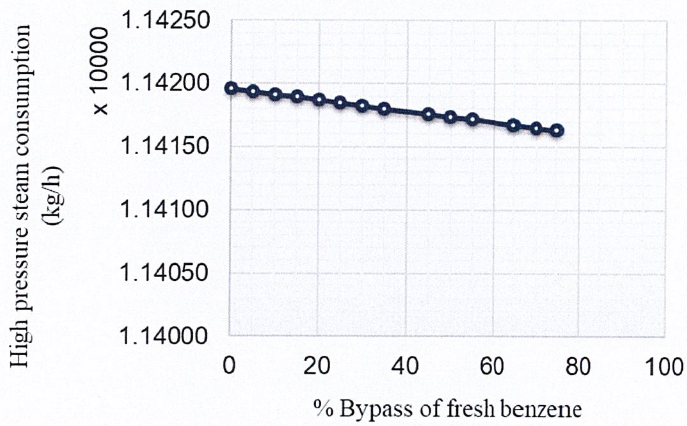


Figure 4.3 The relation between % bypass of fresh benzene feed and the high pressure steam consumption.

In order to maintain the benzene specs at *BOTTOM* and *RECYCLED2*, reflux from the condenser needs to be increased to compensate. The effect of %bypass on reflux flow are shown in the Figure 4.4.(more details are reported in Appendix A2)

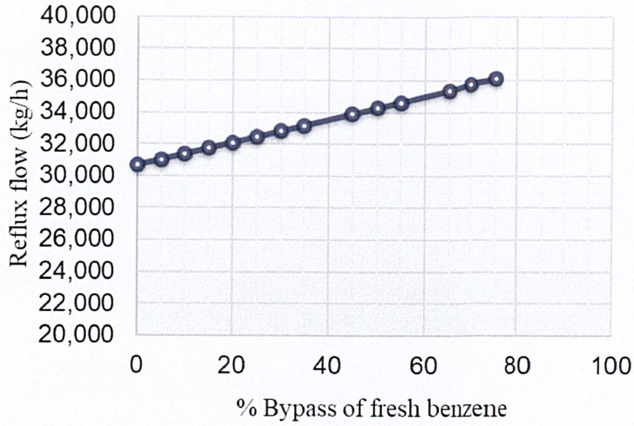


Figure 4.4 The relation between % bypass of fresh benzene feed and the reflux flow rate of benzene column.

4.3.2 Effect of bypassing on water content in *RECYCLE2* stream

Water comes mostly from the fresh benzene feed and can be stripped out in the benzene column. Bypassing fresh benzene results in the increase of water in *RECYCLE2* stream due to the increasing of percentage of bypassing as shown in Figure 4.5. (more details are reported in Appendix A2)

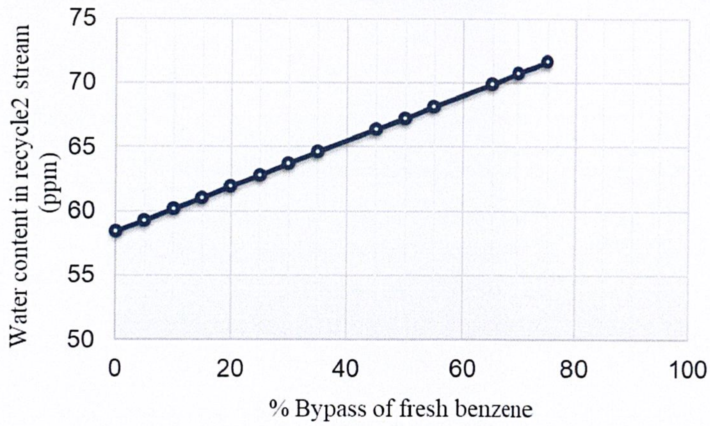


Figure 4.5 The relation between % bypass of fresh benzene feed and water content in *RECYCLE2* stream.

RECYCLE2 stream is sent to alkylation and transalkylation reactors. For the alkylation reactor, water is typically less than 100 ppm. Increasing of water content decreases the temperature of *RECYCLE2* stream, so the temperatures of both reactors need to be heighten to compensate. Moreover, the increase in water content leads to poorer the alkylation selectivity and transalkylation catalyst activity.

4.3.3 Effect of bypassing on the temperature of *RECYCLE2* stream

RECYCLE2 stream is the combination of *RECYCLE* stream that comes from the column and *BYPASS* stream. *RECYCLE* stream is the hot stream with temperature around 105-106 $^{\circ}$C while *BYPASS* stream is the cold stream with temperature around 32°C. After combining these streams to be *RECYCLE2*, temperature of *RECYCLE2* is dropped as shown in Figure 4.6 (more details are reported in Appendix A2). Hence, temperature of *RECYCLE2* is understandably decreased with increasing of bypassing percentage.

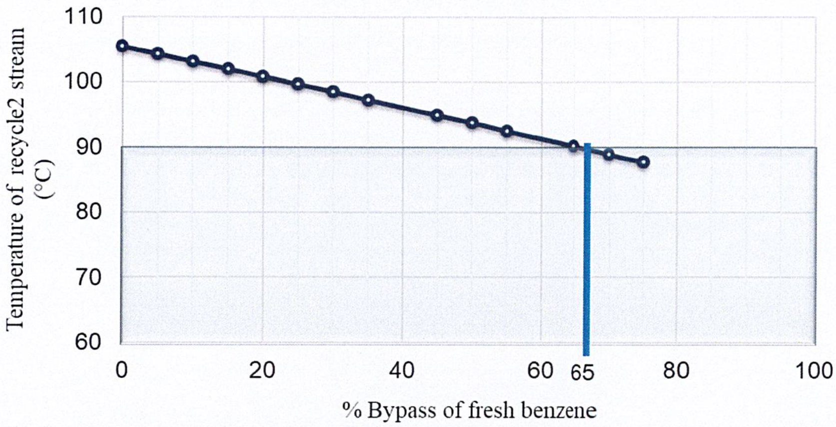


Figure 4.6 The relation between % bypass of fresh benzene feed and the temperature of *RECYCLE2* stream.

Temperature of *RECYCLE2* stream and percentage of bypassing are together plotted in the Figure 4.6. However, the temperature of *RECYCLE2* stream is limited by temperature of alkylation reactor feed. According to the specification, the temperature of *RECYCLE2* stream must be in the range of 90-104°C. Hence, the optimum percentage of bypassing is 65.

4.4 Economic consideration

Saving basis Calculation: high steam 40 bar consumption x High pressure steam (S40 bar) price

- Bypassing fresh benzene feed to the optimum point reduces the high steam 40 bar = 2.85 kg/h
- S40 bar price = 1,039 baht/Ton

Benefit estimation = 2.85 / 1,000 x 24 x 30 x 12 x 1,039

= 25,584.34 baht/year

≈ 25,600 baht/year

From above calculation, it can be seen that bypassing of fresh benzene can save only 25,600 Bath/year. Taking into account the cost saving together with catalyst poisoning, it can be concluded that bypassing of fresh benzene feed is not recommended.

CHAPTER V

CONCLUSIONS

5.1 Conclusions

According to the results reported in the previous chapter, the conclusions are follows.

The model constructed in this work is verified since there is small difference in %error of condition accuracy between the simulation and laboratory data. So, this model can be applied for modifying the bypass.

After modifying the column by bypassing fresh benzene from 0 to 100% with a 5% interval, only 14 from 21 points can be converged with the desired spec which are 0, 5, 10, 15, 20, 25, 30, 35, 45, 50, 55, 65, 70 and 75%. Error was found at 40 and 60% of bypassing. Bypassing more than 75%, the mass conservation of the column fails at specific *Design Spec*. At the maximum bypass (75%), only 3.26 kg/h of high pressure steam is reduced.

High pressure steam consumption depends mainly on the alkylation and transalkylation reactors effluent streams. Thus, bypassing of fresh benzene to benzene recycled stream slightly affects high pressure steam consumption at the reboiler because the alkylation and transalkylation reactors effluents are unchanged and need to be fractionated.

To fractionate benzene at benzene column, fresh benzene influences the reflux of the column. Since bypassing the fresh benzene, the reflux from the condenser must be increased to compensate.

Bypassing the fresh benzene results in the increase of water content in *RECYCLE2* stream affecting poorer alkylation selectivity and transalkylation catalyst activity. Moreover, the temperatures of both reactors need to be heighten to compensate due to the reduction of *RECYCLE2* temperature.

Temperature of *RECYCLE2* stream is limited by temperature of alkylation reactor feed which must be in the range of 90-104°C. Thus, the optimum point that can be bypassed is 65%.

From the benefit estimation, bypassing fresh benzene to the optimum point helps to reduce the consumption of high pressure steam to 2.85 kg/h which is equivalent to 25,600 baht/year. So, there is no significant in steam saving.

In addition, fresh benzene feed may be contaminated by dissolved oxygen, carbonyls, heavies, water and basic nitrogen compound which should be removed. Benzene column helps to remove the impurities as much as possible. Bypassing the fresh benzene at the benzene column leads to the increasing of catalyst deactivation rate.

Therefore, bypassing of the fresh benzene feed directly into the recycled benzene stream is not recommended.

5.2 Further study

1. Change the inlet tray of fresh benzene from stage 11 (11^{th} tray) to stage 12-30 in order to improve the yield in alkylation reactor and to maintain good catalyst activity in transalkylation reactor because more water can be stripped out from the *RECYCLE2* stream.
2. Study the effect of water in *RECYCLE2* stream on high pressure steam consumption because bypassing fresh benzene results in different water contents in *RECYCLE2*, so the high pressure steam consumption may be changed.

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APPENDIX

APPENDIX A1

Actual column

From simulation

Details of Azeotrope

Physical property model: SRK Valid phase: Vapor-Liquid

Mixture investigated for azeotropes at a pressure of 101325 N/SQM11

Azeotropes are found between:

1. Water and Benzene
2. Water and Hexane
3. Water and Toluene
4. Water and Heptane
5. Water and EB
6. Water and Cumene
7. Water and NPB
8. Water and TBB
9. Water and SBB
10. Water and p-cymene
11. Benzene and Hexane

NUMBER OF COMPONENTS: 2		TEMPERATURE 66.31 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.2122
	Benzene	0.7878

NUMBER OF COMPONENTS: 2		TEMPERATURE 47.56 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.2324
	Hexane	0.7676

NUMBER OF COMPONENTS: 2		TEMPERATURE 73.30 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.3233
	Toluene	0.6767

NUMBER OF COMPONENTS: 2		TEMPERATURE 56.06 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.3059
	Heptane	0.6941

NUMBER OF COMPONENTS: 2		TEMPERATURE 76.24 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.3797
	Ethylbenzene	0.6203

NUMBER OF COMPONENTS: 2		TEMPERATURE 75.81 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.3961
	Cumene	0.6039

NUMBER OF COMPONENTS: 2		TEMPERATURE 77.43 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.4148
	NPB	0.5852

NUMBER OF COMPONENTS: 2		TEMPERATURE 74.24 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.3985
	TBB	0.6015

NUMBER OF COMPONENTS: 2		TEMPERATURE 75.08 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.4097
	SBB	0.5903

NUMBER OF COMPONENTS: 2		TEMPERATURE 76.02 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Water	0.4282
	p-Cymene	0.5718

NUMBER OF COMPONENTS: 2		TEMPERATURE 68.93 °C
HOMOGENEOUS		Classification: Saddle
		MASS BASIS
	Benzene	0.0852
	Hexane	0.9148

Table A1.1 Results of actual column outlet streams.

	RECYCLE stream	*BOTTOM* stream	*DRAG* stream	*VENT* stream
Temperature (°C)	105.47	188.92	34	34
Pressure ($kg/cm^2(g)$)	1	1.1	0.518	0.518
Mass flow (kg/h)	70368.28	41654.03	150	150

Table A1.2 Mass fraction of component in the actual column outlet streams.

	RECYCLE stream	*BOTTOM* stream	*DRAG* stream	*VENT* stream
Water	$5.84x10^{-05}$	$4.32x10^{-24}$	0.062	0.0405
Propane	$2.26x10^{-05}$	0	0.0453	0.7338
Butane	$3x10^{-07}$	$1.13x10^{-24}$	0.0005	0.0024
Benzene	0.9316	$3.01x10^{-05}$	0.7258	0.1343
Hexane	$5.45x10^{-04}$	$1.7x10^{-13}$	0.1664	0.089
Toluene	$1.08x10^{-04}$	$1.12x10^{-04}$	$4.43x10^{-08}$	$3.24x10^{-09}$
Heptane	0.0017	$2.41x10^{-04}$	$1.43x10^{-05}$	$2.61x10^{-06}$
Ethylbenzene	$3.37x10^{-05}$	$1.88x10^{-04}$	0	0
Cumene	065.09	788.07	$1.89x10^{-33}$	$2.21x10^{-35}$
NPB	$9.44x10^{-06}$	$1.7x10^{-04}$	0	0
TBB	$5.48x10^{-07}$	$1.52x10^{-05}$	$3.54x10^{-30}$	$3.27x10^{-32}$
SBB	$7.78x10^{-07}$	$3.26x10^{-05}$	0	0
p-Cymene	$5.43x10^{-07}$	$4.33x10^{-05}$	0	0
p-DIPB	$2.49x10^{-06}$	0.2035	0	0
TIPB	$1.26x10^{-11}$	0.006	0	0
2,2DPP	$3.67x10^{-19}$	0.0001	0	0

Table A1.3 Result of actual column condenser.

Temperature (°C)	34
Distillate rate (kg/h)	150
Reflux rate (kg/h)	30672.8
Reflux ratio	204.5
Heat duty (MMkcal/h)	-4.1

Table A1.4 Result of actual column reboiler.

Temperature (°C)	189
Heat duty (MMkcal/h)	4.7

From Laboratory

Table A1.5 Results of outlet streams from laboratory data.

	RECYCLE stream	*BOTTOM* stream
Temperature (°C)	105	4.190
Pressure (kg/cm^2(g))	1	1.1
Mass flow (kg/h)	72113.2	40537.7

Table A1.6 Mass fraction of components in outlet streams from laboratory data.

Mass fraction	Actual data from Laboratory	
	RECYCLE stream	*BOTTOM* stream
Water	5.14×10^{-05}	0
Propane	2.86×10^{-05}	0
Butane	0	
Benzene	9.32×10^{-01}	3.01×10^{-05}
Hexane	1.17×10^{-03}	0
Toluene	1.73×10^{-04}	1.66×10^{-05}
Heptane	6.14×10^{-03}	8.84×10^{-05}
Ethylbenzene	1.92×10^{-05}	1.01×10^{-04}
Cumene	6.01×10^{-02}	8.04×10^{-01}
NPB	5.33×10^{-06}	1.88×10^{-04}
TBB	0	1.64×10^{-05}
SBB	0	3.41×10^{-05}
p-Cymene	0	5.32×10^{-05}
p-DIPB	7.15×10^{-04}	1.95×10^{-01}
TIPB	0	0
2,2DPP	0	0

APPENDIX A2

Modify the column

Table A2.1 Flow of inlet streams after bypassing.

Bypass (%)	*FEED* flow (kg/h)	*EFFLUENT* flow (kg/h)	*BYPASS* flow *(kg/h)*	*FEED2* flow (kg/h)
0	25275.3	86897	0.00	25275.3
5	25275.3	86897	1263.7	24011.6
10	25275.3	86897	2527.5	22747.8
15	25275.3	86897	3791.3	21484
20	25275.3	86897	5055.1	20220.3
25	25275.3	86897	6318.8	18956.5
30	25275.3	86897	7582.6	17692.7
35	25275.3	86897	8846.4	16429
45	25275.3	86897	11373.9	13901.4
50	25275.3	86897	12637.7	12637.7
55	25275.3	86897	13901.4	11373.9
65	25275.3	86897	16429	8846.4
70	25275.3	86897	17692.7	7582.6
75	25275.3	86897	18956.5	6318.8

Table A2.2 Flow of outlet streams after bypassing.

Bypass (%)	*RECYCLE* flow (kg/h)	*RECYCLE2* flow (kg/h)	*BOTTOM* flow *(kg/h)*	*DRAG flow* (kg/h)	*VENT flow* (kg/h)
0	70368.3	70368.3	41654.1	117.2	32.8
5	69105.2	70369	41653.4	117.2	32.8
10	67842.1	70369.7	41652.6	117.1	32.9
15	66579.1	70370.4	41651.9	117.1	32.9
20	65316.1	70371.1	41651.2	117	33
25	64053.	70371.9	41650.5	117	33
30	62789.9	70372.6	41649.8	116.9	33.1
35	61526.9	70373.3	41649	116.9	33.2
45	59000.7	70374.6	41647.7	116.8	33.3
50	57737.7	70375.4	41646.9	116.7	33.3
55	56474.6	70376.1	41646.2	116.7	33.3
65	53948.6	70377.6	41644.7	116.6	33.4
70	52685.5	70378.3	41644	116.5	33.5
75	51422.4	70379	41643.4	116.5	33.5

Table A2.3 Utility and reflux after bypassing.

Bypass (%)	High pressure steam consumption (kg/h)	Heat duty of reboiler (MMcal/h)	Reflux flow (kg/h)	Reflux ratio
0	1.14195 x10^{04}	4.69206	30672.8	204.5
5	1.14193 x10^{04}	4.69197	31025.9	206.8
10	1.14191 x10^{04}	4.69188	31380.4	209.2
15	1.14189 x10^{04}	4.69179	31736.2	211.6
20	1.14187 x10^{04}	4.6917	32093.5	214
25	1.14184 x10^{04}	4.6916	32452	216.3
30	1.14182 x10^{04}	4.69152	32812	218.7
35	1.14180 x10^{04}	4.69142	33173.2	221.2
45	1.14176 x10^{04}	4.69126	33899.8	226
50	1.14174 x10^{04}	4.69116	34264.8	228.4
55	1.14171 x10^{04}	4.69107	34631.3	230.9
65	1.14167 x10^{04}	4.69089	35367.9	235.8
70	1.14165 x10^{04}	4.6908	35738.1	238.3
75	1.14163 x10^{04}	4.69072	36109.6	240.7

Table A2.4 Mass fraction of benzene in outlet streams after bypassing.

Bypass (%)	*RECYCLE* stream	*RECYCLE2* stream	*Bottom* stream
0	9.32×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
5	9.3×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
10	9.29×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
15	9.28×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
20	9.26×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
25	9.25×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
30	9.23×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
35	9.22×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
45	9.19×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
50	9.17×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
55	9.15×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
65	9.11×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
70	9.09×10^{-01}	9.32×10^{-01}	3.01×10^{-05}
75	9.07×10^{-01}	9.32×10^{-01}	3.01×10^{-05}

Table A2.5 Mass fraction of cumene in outlet streams after bypassing.

Bypass (%)	*RECYCLE* stream	*RECYCLE2* stream	*Bottom* stream
0	6.59×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
5	6.71×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
10	6.83×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
15	6.96×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
20	7.1×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
25	7.24×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
30	7.39×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
35	7.54×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
45	7.87×10^{-02}	6.59×10^{-02}	7.89×10^{-01}
50	8.04×10^{-02}	6.6×10^{-02}	7.89×10^{-01}
55	8.22×10^{-02}	6.6×10^{-02}	7.89×10^{-01}
65	8.61×10^{-02}	6.6×10^{-02}	7.89×10^{-01}
70	8.82×10^{-02}	6.6×10^{-02}	7.89×10^{-01}
75	9.03×10^{-02}	6.6×10^{-02}	7.89×10^{-01}

Table A2.6 Water content in outlet streams (ppm) after bypassing.

Bypass (%)	*RECYCLE* stream	*RECYCLE2* stream
0	58.38	58.38
5	58.3	59.27
10	58.22	60.1
15	58.13	61.03
20	58.04	61.92
25	57.95	62.8
30	57.85	63.69
35	57.75	64.57
45	57.54	66.34
50	57.43	67.22
55	57.31	68.11
65	57.06	69.88
70	56.92	70.76
75	56.78	71.65

Table A2.7 Temperature of outlet streams after bypassing.

Bypass (%)	*RECYCLE* flow (kg/h)	*RECYCLE2* flow (kg/h)	*BOTTOM* flow *(kg/h)*	*DRAG flow* (kg/h)	*VENT flow* (kg/h)
0	105.5	105.5	188.9	34	34
5	105.5	104.3	188.9	34	34
10	105.5	103.1	188.9	34	34
15	105.6	102.0	188.9	34	34
20	105.6	100.8	188.9	34	34
25	105.6	99.6	188.9	34	34
30	105.7	98.5	188.9	34	34
35	105.7	97.3	188.9	34	34
45	105.8	94.9	188.9	34	34
50	105.8	93.7	188.9	34	34
55	105.9	92.5	188.9	34	34
65	106.0	90.1	188.9	34	34
70	106.0	88.9	188.9	34	34
75	106.1	87.7	188.9	34	34

In the range of bypassing percentages except at 40%, 60% and more than 75% of bypassing, material and energy balances converged. The example of composition curve at 0% is showed in Figure A2.1

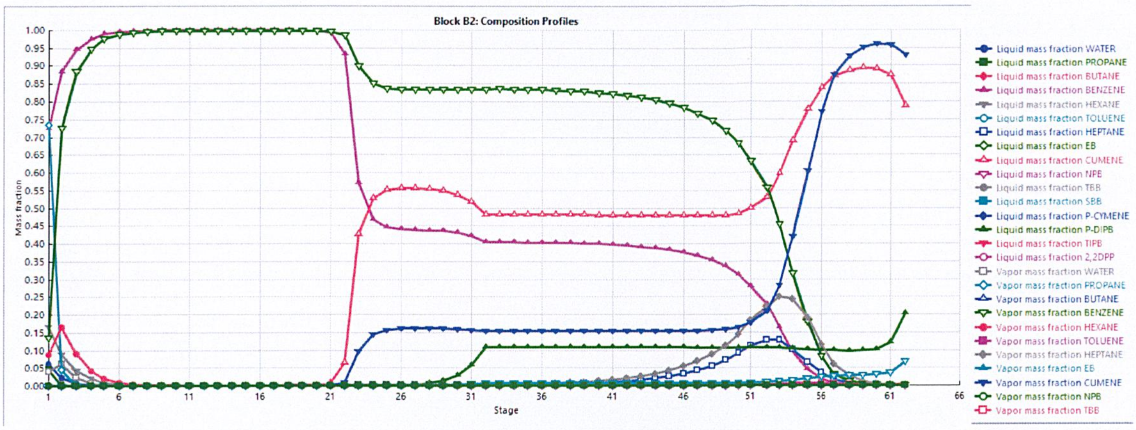

Figure A2.1 Composition profile at 0% bypassing fresh benzene feed.

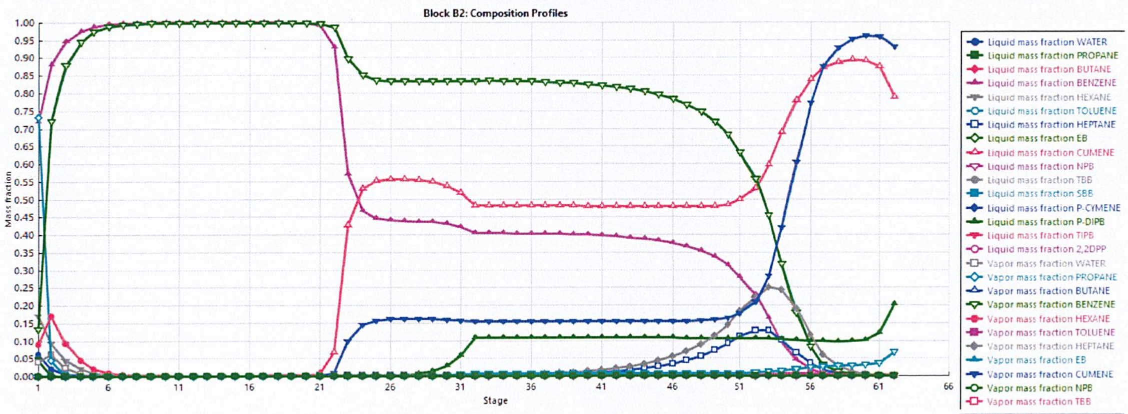

Figure A2.2 Composition profile at 5% bypassing fresh benzene feed.

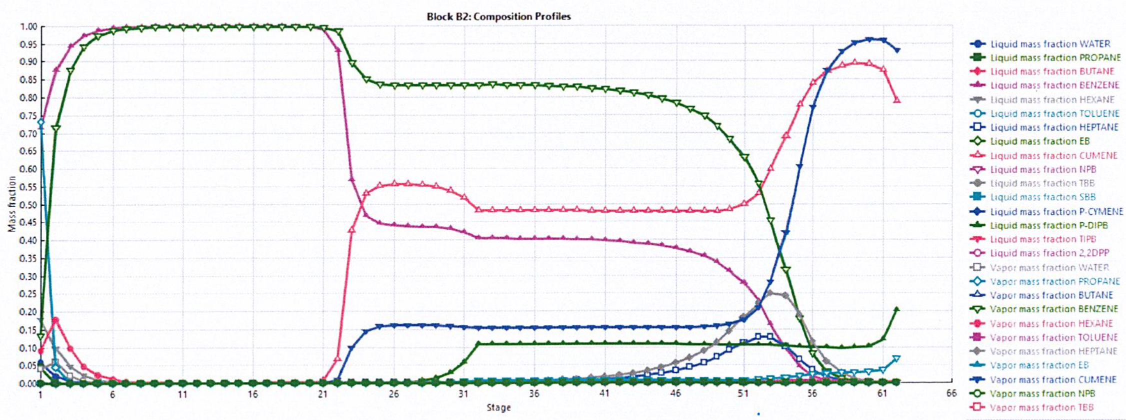

Figure A2.3 Composition profile at 10% bypassing fresh benzene feed.

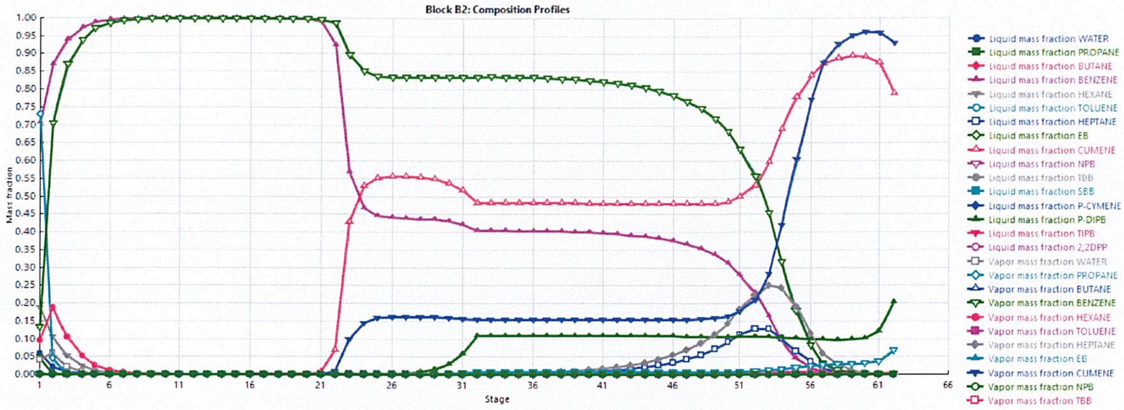

Figure A2.4 Composition profile at 20% bypassing fresh benzene feed.

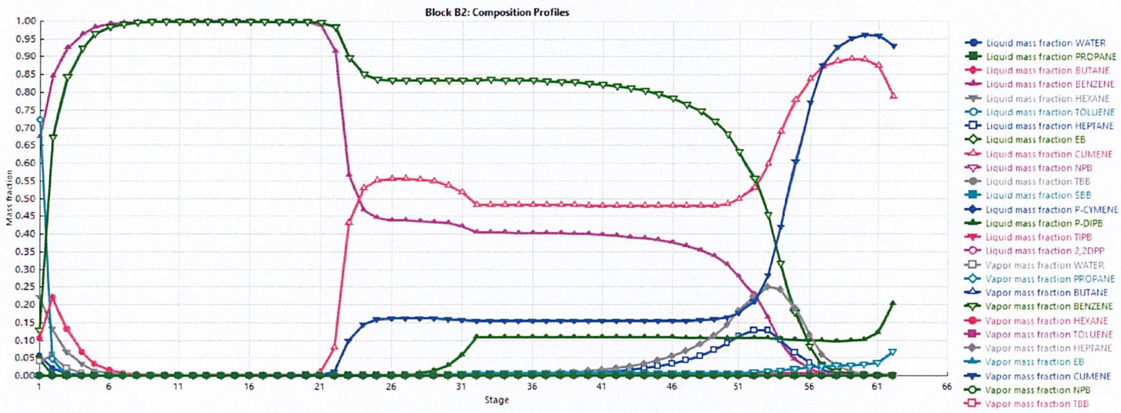

Figure A2.5 Composition profile at 50% bypassing fresh benzene feed.

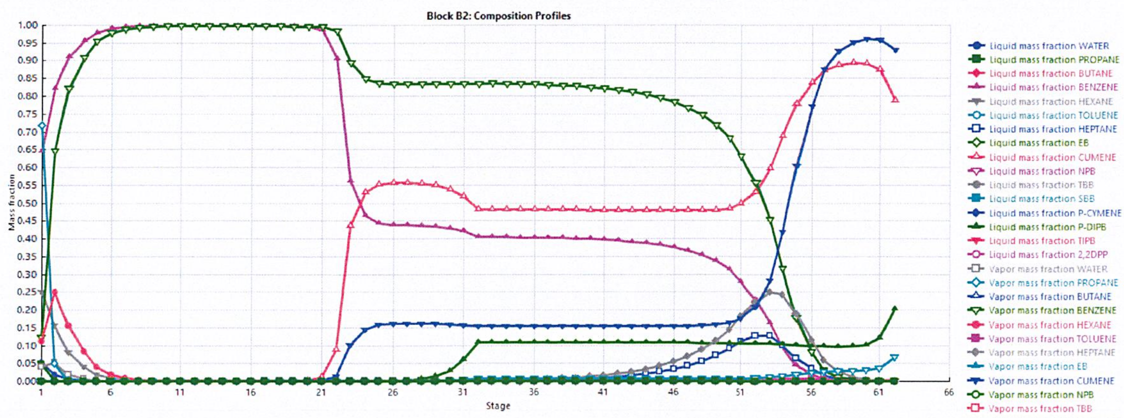

Figure A2.6 Composition profile at 75% bypassing fresh benzene feed.

At 80%-90% of bypassing, material and energy balances fails to converge. The results shown in Figure A2.7 that stages 22, 23, 24, 25, 26, 27, 28, 29, 30 and 31 are dried up.

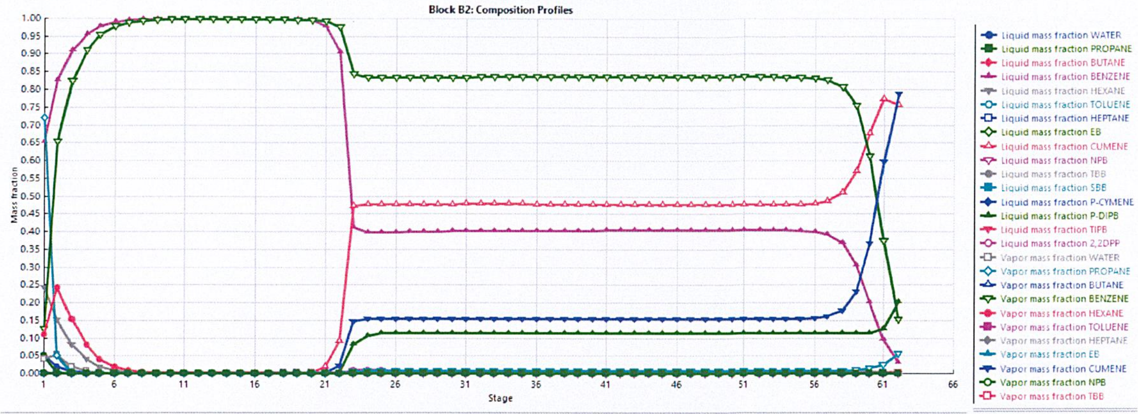

Figure A2.7 Composition profile at 80-90% bypassing fresh benzene feed.

At 95% of bypassing, material and energy balances fails to converge. The results shown Figure A2.8 that stage 22, 23, 24, 25, 26, 27, 28, 29 and 30 are dried up.

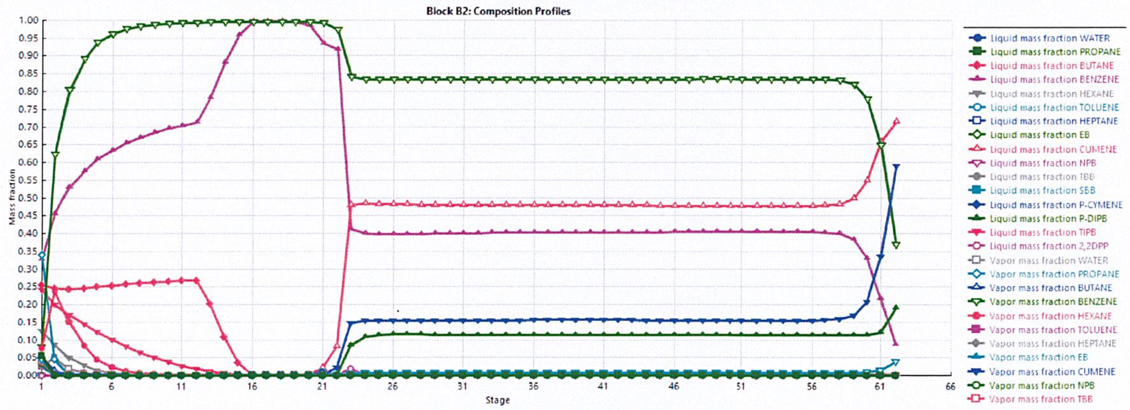

Figure A2.8 Composition profile at 95% bypassing fresh benzene feed.

At 100% of bypassing, material and energy balances fails to converge. The results shown Figure A2.9 that stage 22, 23, 24, 25, 30 and 31 are dried up.

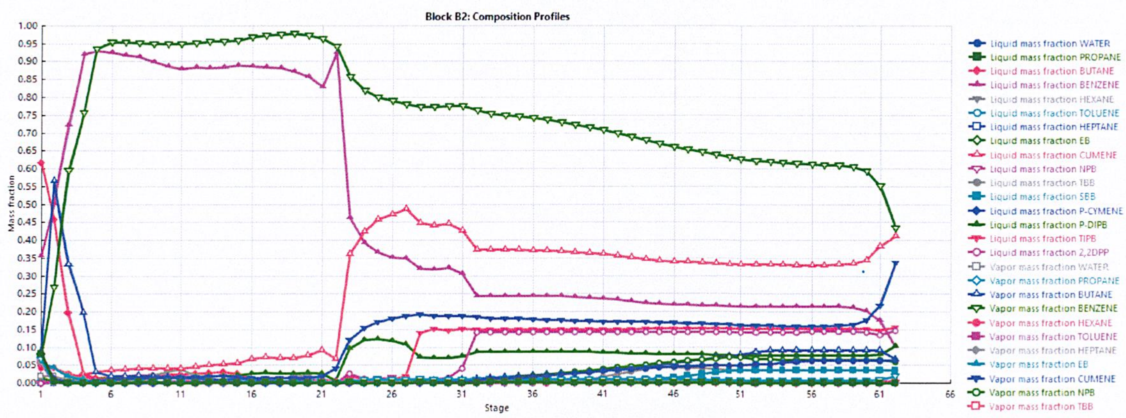

Figure A2.9 Composition profile at 100% bypassing fresh benzene feed.

APPENDIX B

Material Safety Data Sheet

Benzene MSDS

Health	2
Fire	3
Reactivity	0
Personal Protection	H

Section 1: Hazards Identification

Potential Acute Health Effects:

Very hazardous in case of eye contact (irritant), of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:

CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC.

MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast.

TERATOGENIC EFFECTS: Not available.

DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. The substance is toxic to blood, bone marrow, central nervous system (CNS). The substance may be toxic to liver, Urinary System. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 2: First Aid Measures

Eye Contact:

Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention immediately.

Skin Contact:

In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention if symptoms appear.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 3: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 497.78°C (928°F)

Flash Points: CLOSED CUP: -11.1°C (12°F).

Flammable Limits: LOWER: 1.2% UPPER: 7.8%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances:
Highly flammable in presence of open flames and sparks, of heat. Slightly flammable to flammable in presence of oxidizing materials. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:

Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. Explosive in presence of oxidizing materials, of acids.

Fire Fighting Media and Instructions:

Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog.

Special Remarks on Fire Hazards:

Extremely flammable liquid and vapor. Vapor may cause flash fire. Reacts on contact with iodine heptafluoride gas. Dioxygenyl tetrafluoroborate is as very powerful oxidant. The addition of a small particle to small samples of benzene, at ambient temperature, causes ignition. Contact with sodium peroxide with benzene causes ignition. Benzene ignites in contact with powdered chromic anhydride. Vigorous or incandescent reaction with hydrogen + Raney nickel (above 210 C) and bromine trifluoride.

Special Remarks on Explosion Hazards:

Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, di-manganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powerful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

Section 4: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:

Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed.

Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 5: Handling and Storage

Precautions:

Keep locked up. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:

Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 6: Exposure Controls/Personal Protection

Engineering Controls:

Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:

Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:

Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:

TWA: 0.5 STEL: 2.5 (ppm) from ACGIH (TLV) [United States] TWA: 1.6 STEL: 8 (mg/m3) from ACGIH (TLV) [United States] TWA: 0.1 STEL: 1 from NIOSH TWA: 1 STEL: 5 (ppm) from OSHA

(PEL) [United States] TWA: 10 (ppm) from OSHA (PEL) [United States] TWA: 3 (ppm) [United Kingdom (UK)] TWA: 1.6 (mg/m3) [United Kingdom (UK)] TWA: 1 (ppm) [Canada] TWA: 3.2 (mg/m3) [Canada] TWA: 0.5 (ppm) [Canada]Consult local authorities for acceptable exposure limits.

Section 7: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Aromatic. Gasoline-like, rather pleasant. (Strong.)

Taste: Not available.

Molecular Weight: 78.11 g/mole

Color: Clear Colorless. Colorless to light yellow. pH (1% solution/water): Not available.

Boiling Point: 80.1 (176.2°F)

Melting Point: 5.5°C (41.9°F)

Critical Temperature: 288.9°C (552°F)

Specific Gravity: 0.8787 @ 15 C (Water = 1)
Vapor Pressure: 10 kPa (@ 20°C)

Vapor Density: 2.8 (Air = 1) Volatility: Not available.

Odor Threshold: 4.68 ppm

Water/Oil Distribution Coefficient: The product is more soluble in oil; log(oil/water) = 2.1

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Solubility:

Miscible in alcohol, chloroform, carbon disulfide oils, carbon tetrachloride, glacial acetic acid, diethyl ether, acetone. Very slightly soluble in cold water.

Section 8: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.
Conditions of Instability: Heat, ignition sources, incompatibles.

Incompatibility with various substances: Highly reactive with oxidizing agents, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:

Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, dimanganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powerful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 9: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation.

Toxicity to Animals:

WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 930 mg/kg [Rat]. Acute dermal toxicity (LD50): >9400 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 10000 7 hours [Rat].

Chronic Effects on Humans:
CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC.
MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast.
DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. Causes damage to the following organs: blood, bone marrow, central nervous system (CNS). May cause damage to the following organs: liver, Urinary System.
Other Toxic Effects on Humans:
Very hazardous in case of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (female fertility, Embryotoxic and/or foetotoxic in animal) and birth defects. May affect genetic material (mutagenic). May cause cancer (tumorigenic, leukemia)) Human: passes the placental barrier, detected in maternal milk.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. It can be absorbed through intact skin and affect the liver, blood, metabolism,and urinary system. Eyes: Causes eye irritation. Inhalation: Causes respiratory tract and mucous membrane irritation. Can be absorbed through the lungs. May affect behavior/ Central and Peripheral nervous systems (somnolence, muscle weakness, general anesthetic, and other symptoms similar to ingestion), gastrointestinal tract (nausea), blood metabolism, urinary system. Ingestion: May be harmful if swallowed. May cause gastrointestinal tract irritation including vomiting. May affect behavior/Central and Peripheral nervous systems (convulsions, seizures, tremor, irritability, initial CNS stimulation followed by depression, loss of coordination, dizziness, headache, weakness, pallor, flushing), respiration (breathlessness and chest constriction), cardiovascular system, (shallow/rapid pulse), and blood..

Section 10: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 11: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 12: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: Benzene UNNA: 1114 PG: II

Special Provisions for Transport: Not available.

Section 13: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Benzene California prop. 65 (no significant risk level): Benzene: 0.007 mg/day (value) California prop. 65: This product contains the following

ingredients for which the State of California has found to cause cancer which would require a warning under the statute: Benzene Connecticut carcinogen reporting list.: Benzene Connecticut hazardous material survey.: Benzene Illinois toxic substances disclosure to employee act: Benzene Illinois chemical safety act: Benzene New York release reporting list: Benzene Rhode Island RTK hazardous substances: Benzene Pennsylvania RTK: Benzene Minnesota: Benzene Michigan critical material: Benzene Massachusetts RTK: Benzene Massachusetts spill list: Benzene New Jersey: Benzene New Jersey spill list: Benzene Louisiana spill reporting: Benzene California Director's list of Hazardous Substances: Benzene TSCA 8(b) inventory: Benzene SARA 313 toxic chemical notification and release reporting: Benzene CERCLA: Hazardous substances.: Benzene: 10 lbs. (4.536 kg)

Other Regulations:

OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):

CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):

R11- Highly flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes. R45- May cause cancer. R62- Possible risk of impaired fertility. S2- Keep out of the reach of children. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S39- Wear eye/face protection. S46- If swallowed, seek medical advice immediately and show this container or label. S53- Avoid exposure - obtain special instructions before use.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:

Gloves. Lab coat. Vapor respirator. Be sure to use an approved/ certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 14: Other Information

References: http://www.sciencelab.com/msds.php?msdsId=9927339

Material Safety Data Sheet

Cumene MSDS

Health	2
Fire	3
Reactivity	0
Personal Protection	H

Section 1: Hazards Identification

Potential Acute Health Effects:

Very hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:

Very hazardous in case of skin contact (permeator).
CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.
DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs, the nervous system, mucous membranes. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 2: First Aid Measures

Eye Contact:

Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:

After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact:

Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation: Allow the victim to rest in a well-ventilated area. Seek immediate medical attention

Serious Inhalation:

Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:

Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 3: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 424°C (795.2°F)

Flash Points: CLOSED CUP: 36°C (96.8°F). OPEN CUP: 44°C (111.2°F).

Flammable Limits: LOWER: 0.9% UPPER: 6.5%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Flammable in presence of open flames and sparks.

Explosion Hazards in Presence of Various Substances:

Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:

Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 4: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:

Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 5: Handling and Storage

Precautions:

Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. In case of insufficient ventilation, wear suitable respiratory equipment If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes

Storage:

Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

Section 6: Exposure Controls/Personal Protection

Engineering Controls:

Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:

Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:

Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:

TWA: 50 CEIL: 75 (ppm) TWA: 245 CEIL: 365 (mg/m3) Consult local authorities for acceptable exposure limits.

Section 7: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 120.2 g/mole Color: Clear Colorless.

pH (1% solution/water): Not available.

Boiling Point: 152.4°C (306.3°F)

Melting Point: -96°C (-140.8°F)

Critical Temperature: Not available.

Specific Gravity: 0.862 (Water = 1)

Vapor Pressure: 8 mm of Hg (@ 20°C)

Vapor Density: 4.14 (Air = 1)

Volatility: Not available.

Odor Threshold: 1.2 ppm

Water/Oil Distribution Coefficient: The product is more soluble in oil; log(oil/water) = 3.7

Ionicity (in Water): Not available.

Dispersion Properties: Not available.

Solubility: Very slightly soluble in cold water.

Section 8: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No

Section 9: Toxicological Information

Routes of Entry: Dermal contact. Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 1400 mg/kg [Rat]. Acute dermal toxicity (LD50): 12300 mg/kg [Rabbit].

Chronic Effects on Humans: The substance is toxic to lungs, the nervous system, mucous membranes.

Other Toxic Effects on Humans: Very hazardous in case of skin contact (irritant, permeator), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 10: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 11: Disposal Considerations

Waste Disposal

Section 12: Transport Information

DOT Classification: Class 3: Flammable liquid.

Identification: Isopropylbenzene: UN1918 PG: III

Special Provisions for Transport: Marine Pollutant

Section 13: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: Cumene Massachusetts RTK: Cumene TSCA 8(b) inventory: Cumene SARA 313 toxic chemical notification and release reporting: Cumene CERCLA: Hazardous substances.: Cumene

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:
WHMIS (Canada):
CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F).
DSCL (EEC):
R10- Flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes.
HMIS (U.S.A.):
Health Hazard: 2
Fire Hazard: 3
Reactivity: 0
Personal Protection: h
National Fire Protection Association (U.S.A.):
Health: 2
Flammability: 3
Reactivity: 1
Specific hazard:

Protective Equipment:

Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 14: Other Information

References: http://www.sciencelab.com/msds.php?msdsId=9927504

BIOGRAHPY

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