FRAMEWORK FOR INHERENT SAFETY COST EVALUATION

by

NUR HIDAYATUL LIYANA BINTI YAHYA

15120

Dissertation submitted in partial fulfillment of
the requirements for the
Bachelor of Engineering (Hons)
(Chemical)

MAY 2014

Universiti Teknologi PETRONAS
Bandar Seri Iskandar
31750 Tronoh
Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

INTEGRATED COST INDEX FOR INHERENTLY SAFER DESIGN ALTERNATIVES

by

NUR HIDAYATUL LIYANA BINTI YAHYA

A project dissertation submitted to the
Chemical Engineering Programme
Universiti Teknologi PETRONAS
in partial fulfillment of the requirement for the
BACHELOR OF ENGINEERING (Hons)
(CHEMICAL ENGINEERING)

Approved by,

____
(Dr. Risza Binti Rusli)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
MAY 2014

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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(NUR HIDAYATUL LIYANA BINTI YAHYA)

ABSTRACT

Inherently Safer Design (ISD) is an approach in process industry to prevent any loss and injuries especially in the design and operation of facilities that use hazardous chemical. The sole purpose is to minimize the frequency and potential impact of chemical plant incident such as fires, explosion and acute toxic exposure. There are four strategies for designing inherently safer process which is substitute, minimize, moderate and simplify. These strategies can either be to choose only one strategy or to apply all of the strategies best at the preliminary stage in designing a plant. Considering the lifetime cost of a process and its operation, an inherent safety approach can lead to a cost optimal option. However, it is still a big question to chemical industry whether the cost is affordable when applying ISD. Therefore, in this this report, safety and economic evaluation have been made for three alternatives chosen from the MMA process routes. Index used in evaluating safety is Prototype Index for Inherent Safety (PIIS). A framework to evaluate modification cost which comprises material and equipment purchasing cost has been developed for the economic evaluation purpose. These two cost evaluations are made to determine the impact of cost towards the inherent safety implementation. This works has shown that inherently safer design does affect the economic feasibility of a process where the safest design does not necessarily be the cheapest design alternative.

ACKNOWLEDGEMENT

All praise to Allah, the most merciful for giving me the strength and determination in completing this project in Universiti Teknologi PETRONAS. First and foremost I would like to express my deepest gratitude to my supervisor, Dr Risza Rusli for her unconditional guide and support throughout the project. Besides, I would also like to thank Miss Mardhati Zainal Abidin post graduate student under Dr Risza Ruli for helping me in conducting this project. Furthermore, I would like to thank my parents for their continuous support and encouragement in completing this project. Last but not least, I would like to extend my gratitude to anyone who has assisted me directly or indirectly in this project to make my final year project a success.

TABLE OF CONTENT

CERTIFICATION OF APPROVAL i

CERTIFICATION OF ORIGINALITY ii

ABSTRACT iii

ACKNOWLEDGEMENT 1

LIST OF TABLES 4

LIST OF FIGURES 5

CHAPTER 1 : INTRODUCTION 6

1.1 Background 6

1.2 Problem Statement 6

1.3 Objectives and Scope of Study 7

1.3.1 Objectives 7

1.3.2 Scope of study 7

CHAPTER 2 : LITERATURE REVIEW 8

2.1 Chemical Process Safety Strategies 8

2.1.1 Inherent 8

2.1.2 Passive 8

2.1.3 Active 9

2.1.4 Procedural 9

2.2 Inherent Safety Principle 9

2.2.1 Minimize 9

2.2.2 Substitute 10

2.2.3 Moderate 10

2.2.4 Simplify 10

2.3 Case Study on Previous Accident 10

2.3.1 Bhopal Disaster 10

2.3.2 Bayer Crops 11

2.3.3 Flixborough Disaster 12
2.4 Tools for Inherent Safety Evaluation 13
2.4.1 Integrated Inherent Safety Index (I2SI) 13
2.4.2 Inherent Safety Index (ISI) 14
2.4.3 Prototype Index for Inherent Safety (PIIS) 14
2.5 Economic Evaluation 15
2.5.1 Capital Investment 16
2.5.2 Operating Cost 16
CHAPTER 3 : METHODOLOGY/PROJECT WORK 17
3.1 Research Methodology 17
3.2 Process Flow 18
3.2.1 Process Routes 19
3.2.2 Safety Evaluation 19
3.3.3 Economic Evaluation 19
3.3 Gantt chart 21
3.4 Key Milestone 24
CHAPTER 4 : RESULT AND DISCUSSION 25
4.1 Chemical Process Route 25
4.2 Safety Evaluation 27
4.3 Framework to Calculate Modification Cost 28
4.4 Inventories 29
4.4.1 Inventory for Each Process Step 29
4.4.2 Separation Inventory 32
4.4.3 Storage inventory 32
4.5 Modification Cost Evaluation 33
4.6 Relating Inherent Safety to Cost 35
4.6 Problem Encountered 36
CHAPTER 5 : CONCLUSION 38
REFERENCES 39
APPENDICES 41

LIST OF TABLES

Table 1: Chemical and Process score....................15
Table 2: Gantt Chart....................22
Table 3 : Results for MMA routes....................27
Table 4: Totals for each MMA routes....................27
Table 5: ISD cost analysis....................29
Table 6: Flow rate and Inventory for C3 Based Route....................30
Table 7: Flow rate and Inventory for TBA Based Route....................31
Table 8: Flow rate and Inventory for i-C4 Based Route....................31
Table 9: Separation Inventories....................32
Table 10: Raw material storage inventories....................32
Table 11: Product storage inventories....................33
Table 12: Raw Material Cost....................33
Table 13: Equipment Purchasing Cost....................34
Table 14: Cost estimation for MMA routes in US ($)....................34

LIST OF FIGURES

Figure 1: Reactor configuration of cyclohexane process 13
Figure 2: Capital Investment 16
Figure 3: Research Methodology 17
Figure 4: Process flow of project 18
Figure 5: Heuristic of Inherent Safety Cost 20
Figure 6: Project Key Milestone 24
Figure 7: Graph of raw material cost and safety index of MMA routes 35
Figure 8: Graph of equipment purchasing cost and safety index of MMA routes 36

CHAPTER 1
INTRODUCTION

1.1 Background

The concept of inherent safety is not a new concept in chemical industries. It has been recognized long time ago since there were many accidents occurred that time [1]. Until today, the main intention of ISD was always to eliminate or significantly to reduce hazards. However, design alternatives with reduced hazards or even eliminate one hazard may generate or increase the magnitude of others. Therefore, a thorough research must be done first before implementing the ISD concept to the chemical industry.

ISD is considered to be the most robust way to deal with safety and believed to be a subset of green chemistry as well as green engineering. ISD also provides a reliable risk management and able to make the technology in chemical industry to be much simpler and economic than the existing technology[2]. Therefore, this project is focusing on the cost for each process route of the chosen case study.

1.2 Problem Statement

The implementation of ISD to a process with different alternatives shows clear advantages for safety purposes. The reduction of one or more hazards from one process alternative when compared to the other will give significant impact to the process safety. However, when those processes were compared, it was difficult to determine which process is inherently safer. In implementing ISD, business and economic factor must also be considered particularly. Different alternatives have different costing which might improve the process economic or vice versa[3]. Nevertheless, the overall process economics are very complex and impacted by many factors [4]. Thus, economic feasibility is important to be considered during the selection of ISD which is by determining the cost involved.

1.3 Objectives and Scope of Study

1.3.1 Objectives

Referring to the problem statement mentioned, there are few objectives to be achieved in this project which are:

1. To evaluate safety using Prototype Index for Inherent Safety (PIIS)
2. To develop framework to evaluate modification cost for inherently safer design purposes.
3. To evaluate modification cost using the framework.

1.3.2 Scope of study

The study will focus on methyl methacrylate (MMA) process with three different alternatives process routes. PIIS will be used to evaluate the safety of each process routes as PIIS is very significant in the route level. The only cost that will be evaluated in this study is modification cost which will later be compared within the three process routes.

CHAPTER 2

LITERATURE REVIEW

2.1 Chemical Process Safety Strategies

There are four strategies involved in the chemical process safety which are inherent, passive, active and procedural [5]. The most significant and reliable strategies to be used are inherent and passive strategies but all of the strategies need to take into consideration in order to have a broad process safety management program [6]. Each and every strategy will be clearly described below.

2.1.1 Inherent

Inherent approach to safety is to eliminate or reduce hazard by changing the process or condition to less hazardous form for example, using water based latex paints instead of using oil based paints (flammable) which will eventually eliminate the flammable hazard.

2.1.2 Passive

Minimizing the hazards using process or equipment design features is a passive approach where it reduces either the frequency of the hazard or consequences without any active functioning of any device. Hendershot[6] states the example of this approach where a reactor is designed to contain a pressure up to 10 bar to handle the maximum pressure of 5 bar. There is no sensor used to sense high pressure and no moving part are required to contain the 5 bar pressure.

2.1.3 Active

Active safety strategy is purposely designed to sense hazard and response to the hazard. This strategy also designed to prevent incident or to minimize the consequences of an incident. Example of active system is a tank that has a high level interlock that shuts off a pump and closes the feed valve to prevent the tank from overflow. This is differ from the Hazard and Operability Analysis (HAZOP) study where there is a faulty valve installed to safeguard the level inside the tank.

2.1.4 Procedural

Procedural approach involves all the plant procedures such as standard operating procedure, emergency response procedure and management system. This feature does not provide adequate risk management but they will be required to ensure ongoing maintenance and management of active and passive safety system [6] .

2.2 Inherent Safety Principle

According to Peter and Timmerhaus [7], since the inherent safety approach is the most robust and reliable, it is believed that if the inherent approach which is to eliminate hazard is to be implemented alone, other safety strategies may not be required. In order to implement inherent safety design into the processes and plants, there are four principles that are required to take into consideration.

2.2.1 Minimize

Minimize in the context of inherent safety means reduce or minimize the quantity of material or energy enclosed in a process or plant. Example of minimization strategies is a reduction of process inventory by applying a good engineering design to more conservative technology.

2.2.2 Substitute

Substitute principle refers to the replacement of a hazardous material with an alternative that will lessen or eliminate the hazard. This principle is best applied during the preliminary stage of a process for example substituting the raw materials used.

2.2.3 Moderate

Moderate or attenuation means to use material with less hazardous conditions. This moderation principle can be done either by controlling the physical or chemical properties for example by reducing the storage pressure or using a low boiling hazardous material.

2.2.4 Simplify

Eliminating unnecessary complexity or in other words adopting a process as simple as possible is an approach of simplification principle. A simpler process provides a safer and more cost effective than a complex one. An example to this principle is to control hazard by using alarm and safety instrumented system instead of avoiding the hazard by using inherent safer design principles.

2.3 Case Study on Previous Accident

2.3.1 Bhopal Disaster

Around 1 am on Monday, the 3rd of December 1984, in the city of Bhopal, Central India, a poisonous vapour burst from the tall stacks of the Union Carbide pesticide plant. The vapour released was a highly toxic cloud of methyl isocyanate (MIC) which immediately killed more than 5000 people and also killed 15,000 people the following years. Around 100,000 people suffered chronic and devastating illness for which treatment was not effective enough to treat the diseases [8].

The leakage of MIC was said to happen due to the exothermic chemical reaction between MIC and water which lead to a major increase in pressure and heat inside a storage tank. Investigation said that a faulty valve had allowed one ton of water for cleaning internal pipes to mix with forty tons of MIC. The gas flare safety system was out of service for three months. As the gas was released, a weak wind which frequently changed directions, helped the gas to cover more area in just one hour [9].

The major concern in this disaster was the inherent safety of the plant itself. The plant was said to be inherently unsafe. Bhopal disaster had released MIC gas which was neither a raw material nor a finished product, but it was an intermediate reaction in a process step. The chemical should have not been stored in large quantities. Besides, there is other alternative way of making the final product which is to use carbaryl. The usage of carbaryl will change the process route and will not produce MIC. If this alternative has been used, the plant will be inherently safer [10].

2.3.2 Bayer Crops

Bayer Crops incident occurred in August 28, 2008 where 2,200 gallons of flammable solvents of methyl isocyanate(MIC) and toxic insecticide residue sprayed onto the road and into the unit and immediately erupted in flames as several electrical cables or sparks from steel debris striking the concrete ignited the solvent vapour [11]. Two people were killed and eight people were injured in the accident.

An investigation was conducted by the U.S. Chemical Safety and Hazard Investigation Board found that debris from the blast hit the shield surrounding MIC storage tank and have struck a relief valve vent pipe and caused the release of 6,700 gallon methyl isocyanate (MIC) to the atmosphere. Besides MIC, methomyl and solvent were also released. The incident occurred during the first methomyl restart where the methomyl containing solvent was pumped into the residue treater before the vessel was pre-filled

with clean solvent and heated to the required minimum operating temperature specified in the operating procedure. The gas then evolved from the runaway decomposition reaction of methomyl and finally the residue treater violently exploded [11].
On the night of the incident, MIC air monitoring devices in and near the Methomyl-Larvin unit were not in operation. Besides, four gas air monitors worn by emergency responders did not detect hazardous chemical in the air near the unit [11]. In 2011, Bayers CropScience performed hazard and safety assessments which resulted in MIC inventories reduction, elimination of aboveground MIC storage and adoption of various safety measures. However, these assessment have not adopted inherently safer processes with poor management of change and isolation policy [12].

2.3.3 Flixborough Disaster

The flixborough disaster was the UK's largest explosion in the chemical industry happened on the 1st June 1974 where it killed 28 people, injuries to 89 people and destruction of the plant. The incident released cyclohexane at 0.96 MPa and between 150 to 155^{o}C[13].

The explosion was initiated during start up while the cyclohexane feedstock inerted with nitrogen under hot recycle through reactor train, R1 to R6 (as shown in figure below). Before the accident, the fifth reactor, R5 was removed because of a leakage. Therefore, a 20 inch pipe was introduced into this process to bypass the leaking reactor 5, R5 to form a bridge connecting R4 to R6. The 20 inch bypass system suddenly ruptured and released a large quantity of cyclohexane. Cyclohexane formed a flammable mixture and subsequently found a source of ignition [14].

Following the investigation, the presence of a large inventory of cyclohexane has contributed to the release of such a large amount of cyclohexane. Besides, the poor design of 20 inch pipe as well as failure to comply with both safety and design requirements would also be the reason. If the concept of inherent safety was implemented, for example, reducing the inventory, the disruption may not be as huge as what had happened [8].

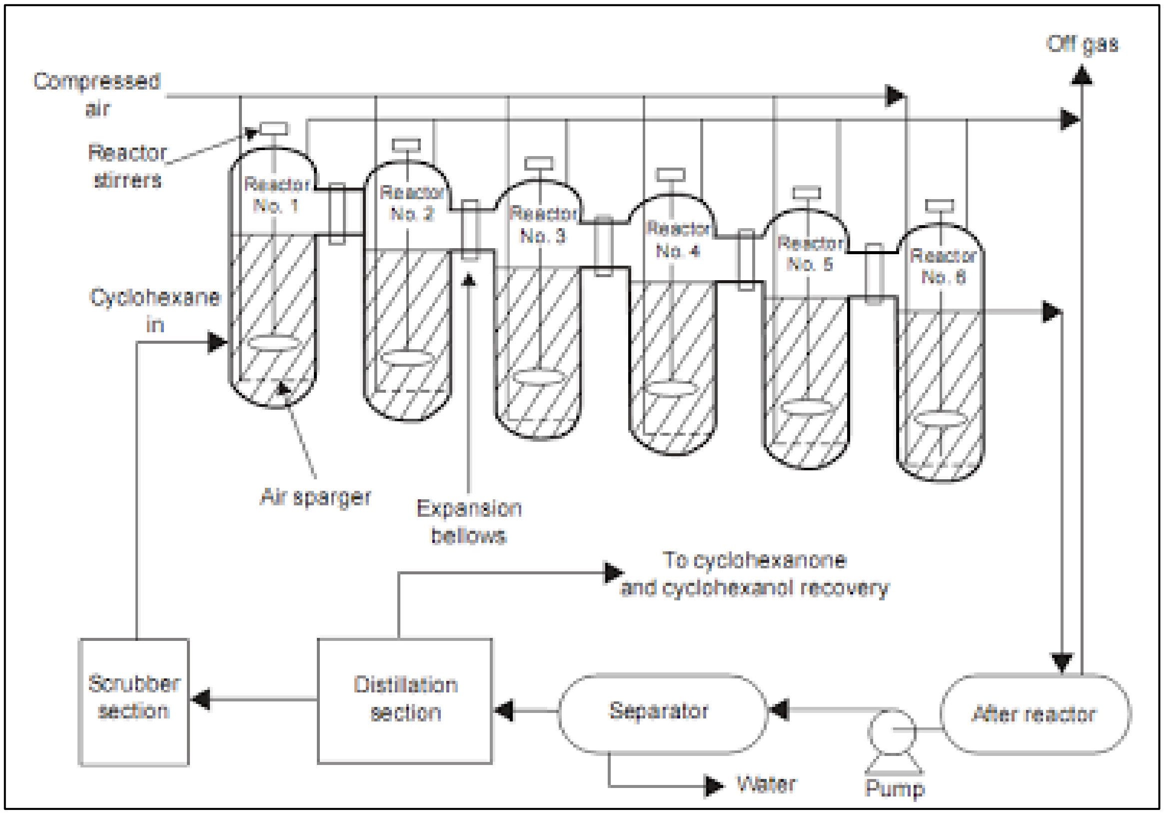


Figure 1: Reactor configuration of cyclohexane process

2.4 Tools for Inherent Safety Evaluation

2.4.1 Integrated Inherent Safety Index (I2SI)

I2SI intended to consider the life cycle of the process with economic evaluation and hazard potential identification for each option that was developed by Faisal and Amyotte in 2004 [15]. This index comprises of sub-indices to account for hazard potential and inherent safety potential as well as the economic potential of the option.

2.4.2 Inherent Safety Index (ISI)

ISI was developed to consider larger scope of process step such as the separation unit and storage unit [16]. The ISI evaluation can be estimated by using physical or chemical properties of compound present or based on operating condition of the process itself. ISI is based on the evaluation of 12 parameters and consist of two main index groups. The two index groups include Chemical Inherent Safety Index and Process Inherent Safety Index which describes the chemical aspect and process related aspect. The parameters involves are

1. Heat of the main reaction
2. Heat of the side reaction
3. Chemical interaction
4. Inventory
5. Process temperature
6. Process pressure
7. Flammability
8. Explosiveness
9. Toxicity
10. Corrosiveness
11. Equipment
12. Process structure

2.4.3 Prototype Index for Inherent Safety (PIIS)

PIIS is the first index published for evaluating the inherent safety in the preliminary stage by Edward and Lawrence in 1996 [17] with the intention to analyze the process route chosen for example inventories and the raw materials used. PIIS is calculated as a sum of Chemical score and a Process Score. These two scores are tabulated in the Table 1.

Table 1: Chemical and Process score

Chemical Scores	Process Scores
• Inventories • Flammability • Explosiveness • Toxicity	• Temperature • Pressure • Yield

2.5 Economic Evaluation

Economic factor is one of the major factors in designing a process plant. According to Seo, economic evaluation should be performed for process optimization [18]. Several costs should be taken into consideration in order to make a decision for the best design alternatives. The lower the costs, the better the performance of the chemical process plant [19]. It is important to determine the overall cost of the designed process alternatives to decide whether to abandon or to proceed with commissioning the project[20].

According to Deddis, in order to determine the economic performance for new process plants or modifications to existing process plant, the cash flow across the entire lifecycle of the project must be considered [4]. This is to ensure that the process plant is economically viable and sustainable. There are two main categories of costs that must be taken into account in evaluating the economics which are the capital investment and operating costs. Capital investment is the initial cost for purchasing purposes whereas the operating costs are the ongoing cost of the operation [4].

2.5.1 Capital Investment

The capital investment is divided into two elements which are fixed capital and working capital. Fixed capital is the cost for purchasing and installing all the equipment requires. Fixed capital can be divided into two cost which is direct cost and indirect cost. Example of direct cost is raw material cost whereas the example for indirect cost is administration cost. Meanwhile for the working capital, it is the cost required to operate the plant. Diagram below shows the division of capital investment.

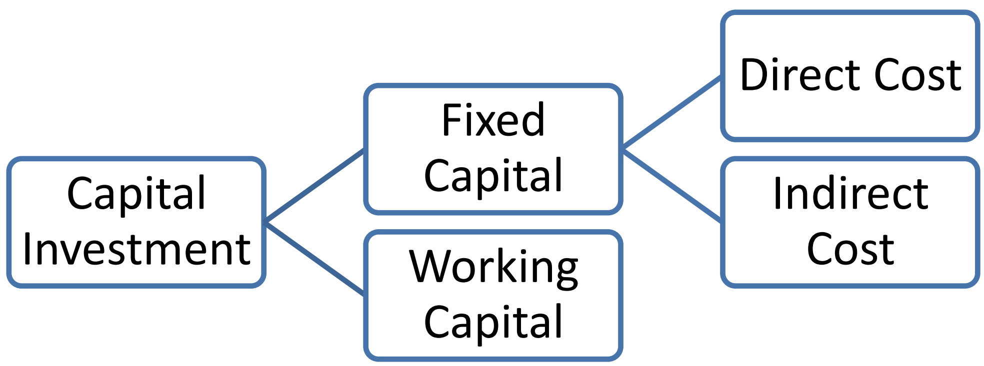


Figure 2: Capital Investment

2.5.2 Operating Cost

Operating cost is the sum of the manufacturing costs and the general administrative expenses where the manufacturing costs consist of direct production costs, fixed cost as well as plant overhead. The management salaries, legal fees, research and development fees are the example of the general administrative expenses.

CHAPTER 3

METHODOLOGY/PROJECT WORK

3.1 Research Methodology

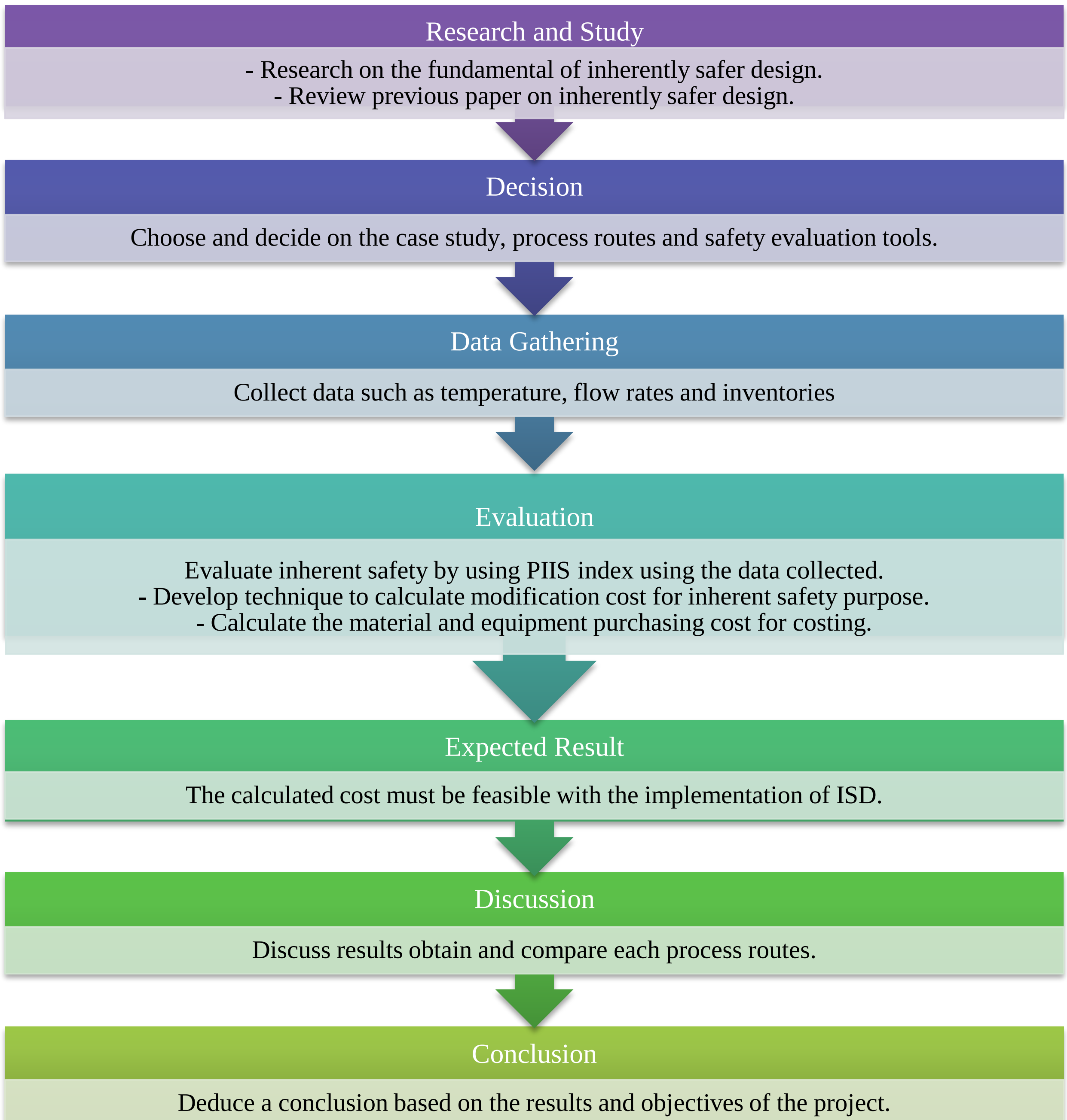


Figure 3: Research Methodology

3.2 Process Flow

In order to ease the project work, a process flow is developed as the methodology of this project. Figure 2 shows the process flow of the project.

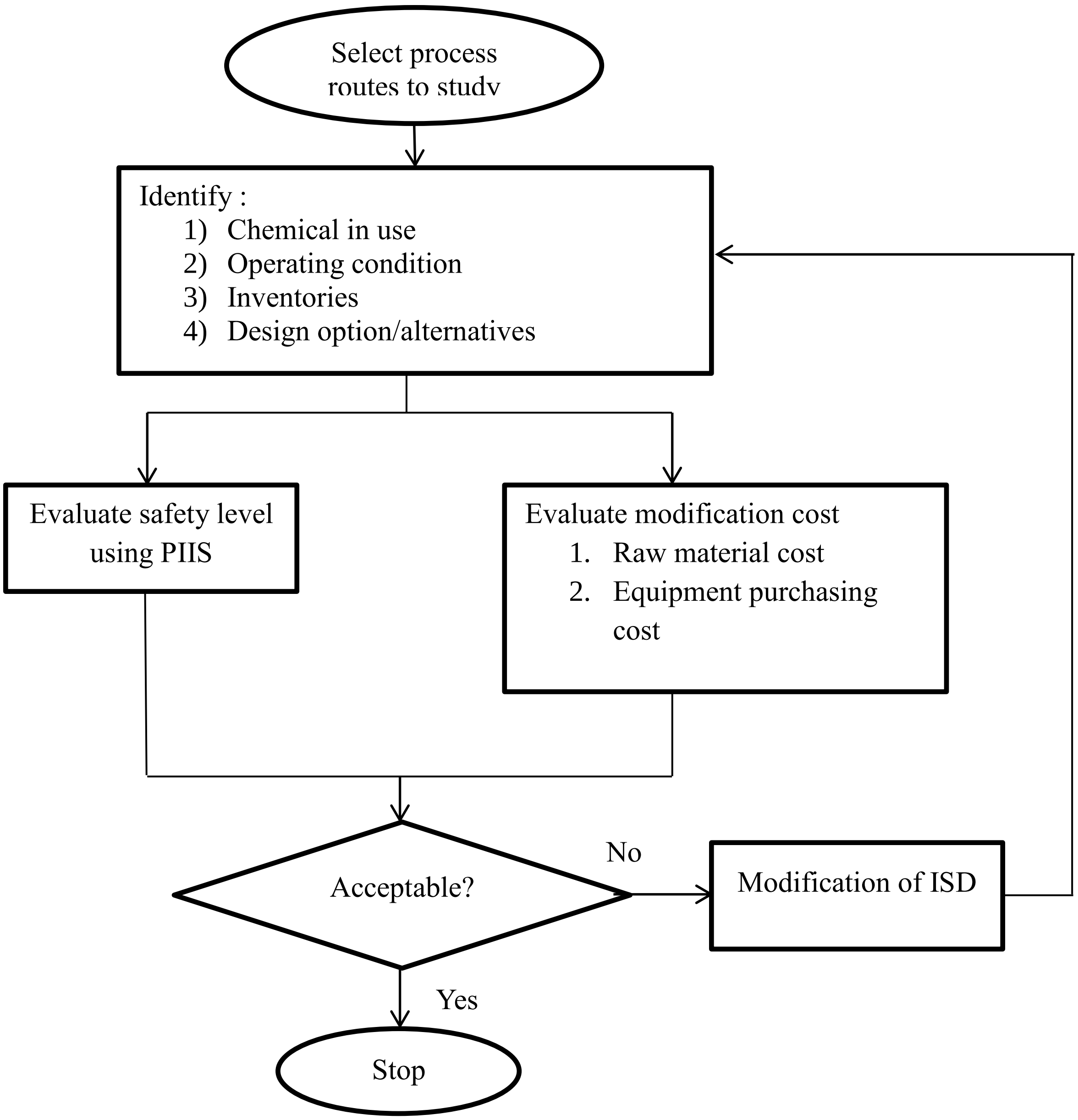


Figure 4: Process flow of project

3.2.1 Process Routes

This project focuses only on three process routes of the MMA case study. The process routes chosen in this project are Propylene based route (C3), Tertiary Butyl Alcohol based route (TBA) and Isobutylene based route (iC4). In order to study the inherent safety, few factors were identified which are the chemical used, operating condition, inventories as well as design alternatives.

3.2.2 Safety Evaluation

Next step is to evaluate safety and modification cost. Since there is already a published paper by Lawrence [17] which uses Prototype Index for Inherent Safety (PIIS) as a tool for safety evaluation on MMA case study, the safety evaluation result is directly used in this project.

3.3.3 Economic Evaluation

In this economic evaluation part, modification cost that comprises raw material cost and modification cost are calculated. Both costs were decided based on the heuristic flow of inherent safety as shown in Figure 5. A framework to calculate the modification cost is developed based on the heuristic flow.

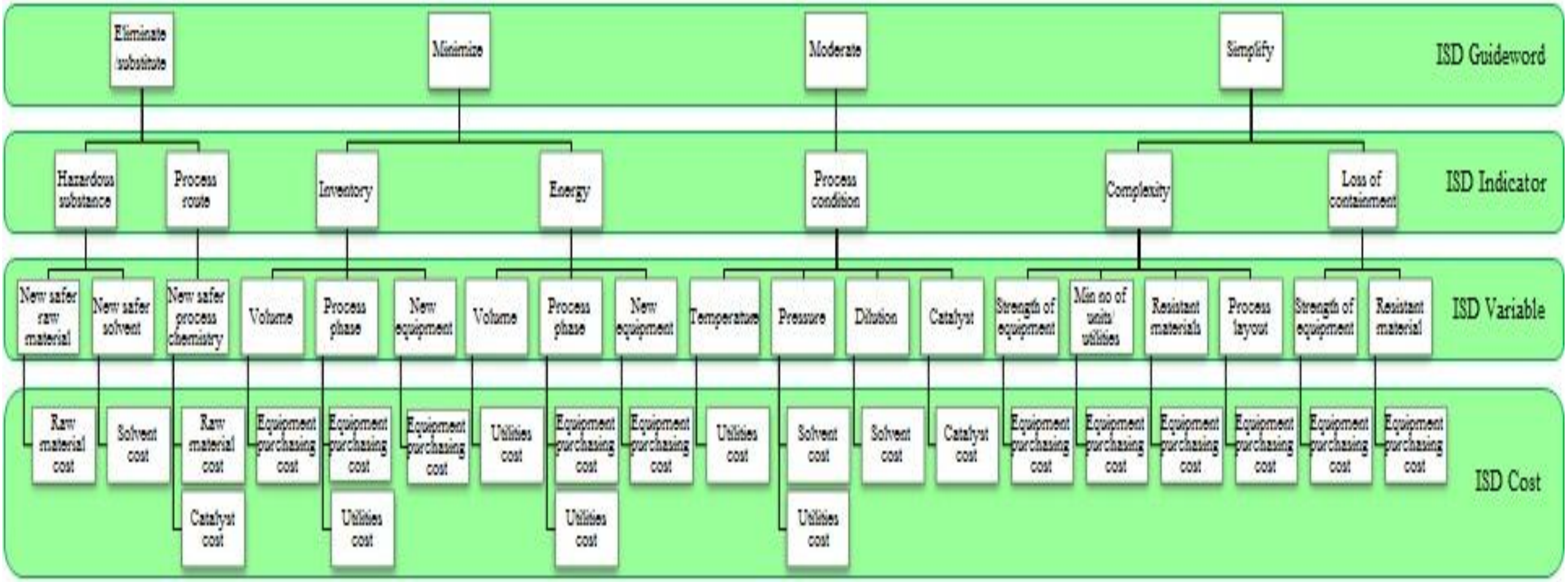


Figure 5: Heuristic of Inherent Safety Cost

3.3 Gantt chart

Gantt chart is produced in order to ensure the objectives of the project can be achieved within the proposed time frame. The gantt chart of the present project is shown in Table below.

Table 2: Gantt Chart

	Detail/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
1	First meeting with coordinator																												
2	First meeting with supervisor																												
3	Preliminary research work and preparing proposal																												
4	Submission of extended proposal							x																					
5	Proposal defense									x																			
6	Collecting data of the chosen case study.																												
7	Submission of interim draft report													x															
8	Submission of final interim report														x														
9	Evaluate safety using PIIS																												
10	Develop technique for cost evaluation																												
11	Submission of progress report																						x						
12	Compilation and analysis of data																												
13	Pre-SEDEX																									x			
14	Submission of draft report																										x		
15	Submission of dissertation (soft bound)																										x		

16	Submission of technical paper																									x		
17	Oral presentation																										x	
18	Submission of dissertation (hard bound)																											x

3.4 Key Milestone

The milestone for the present research is shown in Figure 6.

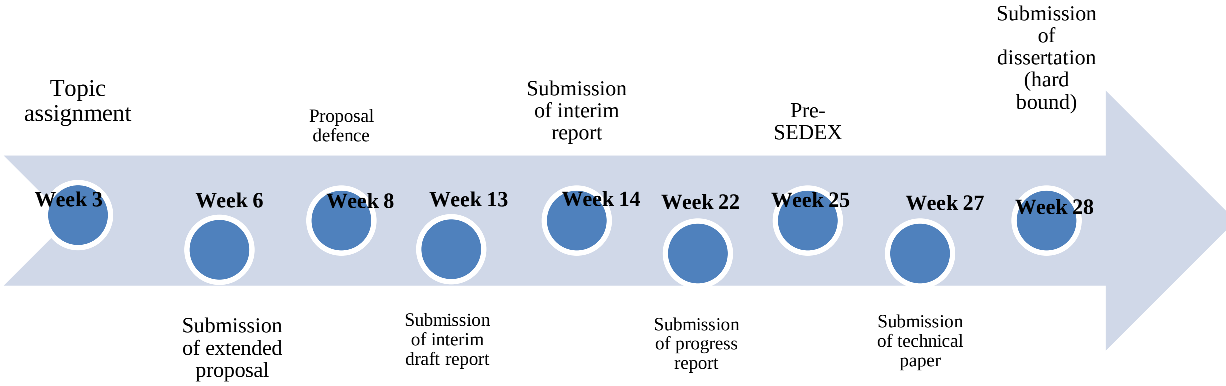


Figure 6: Project Key Milestone

CHAPTER 4

RESULT AND DISCUSSION

4.1 Chemical Process Route

As mention in the first part of this report, MMA routes will be used in this project. Three MMA process routes have been chosen from the previous case study. The following are the MMA route of the three chosen process routes taken from the Lawrence previous research [17].

<u>MMA route 1: Propylene based route (C3)</u>

Step 1:

$CH_3CHCH_2 + CO + HF \longrightarrow (CH_3)_2CHCOF$

Propylene + Carbon Monoxide + Hydrogen Fluoride $\longrightarrow$ Isobutyl Fluoride

Step 2:

$(CH_3)_2CHCOF + H_2O \longrightarrow (CH_3)_2CHCOOH + HF$

Isobutyl Fluoride + Water $\longrightarrow$ Isobutryic Acid +Hydrogen Fluoride

Step 3:

$2(CH_3)_2CHCOOH + O_2 \longrightarrow 2CH_2{=}C(CH_3)COOH + 2H_20$

Isobutyric Acid + Oxygen $\longrightarrow$ Methacyclic Acid + Water

Step 4:

$CH_2{=}C(CH_3)COOH + CH_3OH \longrightarrow CH_2{=}C(CH_3)COOCH_3 + H_2O$

Methacrylic Acid + Methanol $\longrightarrow$ Methyl Methacrylate + Water

MMA route 2: Tertiary Butyl Alcohol based route (TBA)

Step 1:

$(CH_3)_3COH + O_2 \longrightarrow CH_2CCH_3CHO + 2H_2O$

Tertiary Butyl Alcohol + Oxygen ⟶ Methacrolein + Water

Step 2:

$2CH_2CCH_3CHO + O_2 \longrightarrow 2CH_2CCH_3COOH$

Methacrolein + Oxygen ⟶ Methacrylic Acid

Step 3:

$CH_2{=}C(CH_3)COOH + CH_3OH \longrightarrow CH_2{=}C(CH_3)COOCH_3 + H_2O$

Methacrylic Acid + Methanol ⟶ Methyl Methacrylate + Water

MMA route 3: Isobutylene based route (i-C4)

Step 1:

$(CH_3)_2CCH_2 + O_2 \longrightarrow CH_2CCH_3CHO + H_2O$

Isobutylene + Oxygen ⟶ Methacrolein + Water

Step 2:

$2CH_2CCH_3CHO + O_2 \longrightarrow 2CH_2CCH_3COOH$

Methacrolein + Oxygen ⟶ Methacrylic Acid

Step 3:

$CH_2{=}C(CH_3)COOH + CH_3OH \longrightarrow CH_2{=}C(CH_3)COOCH_3 + H_2O$

Methacrylic acid + Methanol ⟶ Methyl Methacrylate + Water

4.2 Safety Evaluation

Table 3 and 4 shows the safety evaluation for MMA process routes taken from a research paper written by Lawrence. The smallest score indicate the safest route. Based on the evaluation, it was clearly shown that TBA alternative route is the safest route among the three routes since it gathered the smallest scores between all the steps.

Table 3 : Results for MMA routes

TOTAL NUMBER OF POSSIBLE DEATHS (F&E) AND LETHAL DOSES (TOXIC)							
		REACTION STEPS		SEPARATION STEPS		STORAGE STEPS	
ROUTE	STEP	F&E	TOXIC	F&E	TOXIC	F&E	TOXIC
C3	1	1	-	1	-	51	
	2	1	1	1	1	N/S	N/S
	3	1	1	2	1	-	-
	4	1	1	2	1	26	3
TOTAL		4	3	6	3	77	3
TBA	1	1	1	N/S	N/S	11	11
	2	1	1	1	1	-	-
	3	1	1	2	1	26	3
TOTAL		3	3	3	2	37	14
i-C4	1	1	1	1	1	59	-
	2	1	1	1	1	-	-
	3	1	1	2	1	25	3
TOTAL		3	3	4	3	84	3

*F&E means fire and explosion

*'N/S' means no separation

*'-' means no data available

Table 4: Totals for each MMA routes

	PROCESS			STORAGE			TOTAL		
ROUTE	F&E	TOXIC	TOTAL	F&E	TOXIC	TOTAL	F&E	TOXIC	TOTAL
C3	10	6	16	77	3	80	87	9	96
TBA	6	5	11	37	14	51	43	19	62
i-C4	7	6	13	84	3	87	91	9	100

Based on Table 4, as discussed in the Lawrence paper, the storage score is much higher than that of process score. This is due to the large difference in the inventories value calculated for both process and storage step. In both steps, TBA based route has the lowest scores compared to C3 and iC4 based route. This is due to the inventories as well as the properties of the chemical used in the process.

4.3 Framework to Calculate Modification Cost

The second objective in this project is to develop a framework to calculate the modification cost. Referring to the material from inherently safer design study [5], a heuristic flow diagram of inherent safety cost as shown in Figure 6 was developed. By using this heuristic flow diagram of inherent safety cost, the author has come out with the cost that will affect the inherent safety cost. Besides, the heuristic flow diagram has made it easier for the author to alter the modification cost.

Table 5 is the result from the analysis of ISD cost by using Figure 5 as a guideline. This table shows the cost that need to be calculated for the economic evaluation purpose. Based on this table, the cost that is to be calculated is the raw material cost, equipment purchasing cost and utilities cost. These costs are considered to be the modification cost.

Table 5: ISD cost analysis

ISD Guideword	ISD Indicator	ISD Variable	ISD Cost
Eliminate/Substitute	Process Routes	New Safer Process Chemistry	Raw Material Cost
Minimize	Inventories	Volume	Equipment purchasing cost
		Process Phase	-Equipment purchasing cost -Utilities cost
Moderate	Process Condition	Temperature	Utilities cost
		Pressure	-Utilities cost

4.4 Inventories

In order to determine the cost of purchasing equipment, it is necessary to calculate the inventory of reaction step, separation as well as storage. The reaction inventory is calculated for all the steps in all MMA alternative routes chosen. Meanwhile, for the separation inventory, only inventory for the purification process for each alternatives route is calculated. Last but not least, storage inventory is calculated for raw material storage and product storage.

4.4.1 Inventory for Each Process Step

The inventory of each process steps are calculated based on few assumptions which is:

Assumption:

- Annual throughput = 50,000 ton/year
- Average production rate = 8150 hr/year (Doughlas,1987)
- Production flow rate = 6.13 ton/hr
- Hold up, H = 1 hour

Propylene (C3) Based Route

Table 6: Flow rate and Inventory for C3 Based Route

	Yield(%)	Species	Chemical formula	n	M	F(t/hr)	I(t)
Step 4	75.00	Methacrylic Acid	C4H6O2	1	86	7.03	7.03
		Methanol	CH4O	1	32	2.62	2.62
		Methyl Methacrylate	C4H8O2	1	100	8.17	8.17
		Water	H2O	1	18	1.47	1.47
Step 3	70.50	Isobutyric Acid	C4H8O2	2	88	10.20	10.20
		Oxygen	O2	1	32	1.85	1.85
		Methacrylic Acid	C4H6O2	2	86	9.97	9.97
		Water	H2O	2	18	2.09	2.09
Step 2	96.20	Isobutyrl Fluoride	C4H7OF	1	90	10.85	10.85
		Water	H2O	1	18	2.17	2.17
		Isobutyric Acid	C4H8O2	1	88	10.61	10.61
		Hydrogen Fluoride	HF	1	20	2.41	2.41
Step 1	94.50	Propylene	C3H6	1	42	5.36	5.36
		Carbon Monoxide	CO	1	28	3.57	3.57
		Hydrogen Fluoride	HF	1	20	2.55	2.55
		Isobutyrl Fluoride	C4H7OF	1	90	11.48	11.48

Tertiary Butyl Alcohol (TBA) Based Route

Table 7: Flow rate and Inventory for TBA Based Route

	Yield(%)	Species	Chemical formula	n	M	F(t/hr)	I(t)
Step 3	83.00	Methacrylic Acid	C4H6O2	1	86	6.35	6.35
		Methanol	CH4O	1	32	2.36	2.36
		Methyl Methacrylate	C4H8O2	1	100	7.39	7.39
		Water	H2O	1	18	1.33	1.33
Step 2	57.75	Methacrolein	C4H6O	2	70	8.95	8.95
		Oxygen	O2	1	32	2.05	2.05
		Methacrylic Acid	C4H6O2	2	86	11.00	11.00
Step 1	75.00	Tertiary Butyl Alcohol	C4H10O	1	74	12.62	12.62
		Oxygen	O2	1	32	5.46	5.46
		Methacrolein	C4H6O	1	70	11.94	11.94
		Water	H20	2	18	6.14	6.14

Isobutylene (i-C4) Based Route

Table 8: Flow rate and Inventory for i-C4 Based Route

	Yield(%)	Species	Chemical formula	n	M	F(t/hr)	I(t)
Step 3	75.00	Methacrylic Acid	C4H6O2	1	86	7.03	7.03
		Methanol	CH4O	1	32	2.62	2.62
		Methyl Methacrylate	C5H8O2	1	100	8.17	8.17
		Water	H2O	1	18	1.47	1.47
Step 2	57.75	Methacrolein	C4H6O	2	70	9.91	9.91
		Oxygen	O2	1	32	2.26	2.26
		Methacrylic Acid	C4H6O2	2	86	12.17	12.17
Step 1	41.80	Isobutylene	C4H8	1	56	18.96	18.96
		Oxygen	O2	1	32	10.83	10.83
		Methacrolein	C4H6O	1	70	23.70	23.70
		Water	H2O	1	18	6.09	6.09

These inventories calculation is very important in preliminary design stage to determine a safer process. A low inventory at every reaction step will require small reactor which is less costly and much safer. Based on the inventories calculation shown in the table above, TBA route shows the lowest inventories value among all with only three process step. Meanwhile, the inventories for i-C4 route are the highest among all which is 23.7 ton in the first step, 12.17 ton in the second step and 8.17 ton in the last step. In order to promote safer process, a lower value of inventories in the every step is required so that the size of the processing equipment in the next process will be much smaller.

4.4.2 Separation Inventory

Separation inventory is calculated to determine the cost of distillation column. In this case study, separation inventory involves only the purification of MMA with the assumption of 99% of purity.

Table 9: Separation Inventories

Route	MMA inventory(t)	Water Inventory(t)
C3	8.0883	1.4553
TBA	7.3161	1.3167
i-C4	8.0883	1.4553

4.4.3 Storage inventory

Assumption = 14days of storage

Table 10: Raw material storage inventories

Raw Material Storage	Storage Inventories(t)	Remark
Propylene	-	Highly flammable
Tertiary Butyl Alcohol	4239.75	
Isobutylene	6370.86	

Table 11: Product storage inventories

Route	Product Storage	Storage Inventories(t)
C3	Methyl Methacrylate(MMA)	2746.24
TBA	Methyl Methacrylate(MMA)	2481.54
i-C4	Methyl Methacrylate(MMA)	2746.24

Based on Table 10, only tertiary butyl alcohol (TBA) and isobutylene (iC4) will be stored in a storage tank as propylene is a highly flammable chemical. TBA has a lower storage inventory than iC4, whereas based on Table 11; TBA has the lowest product storage inventory of MMA compared to C3 and iC4. Thus it is safer to use TBA as a raw material compared to C3 and iC4. This is because, if the storage inventory of any chemical is large, it may cause a large number of accidents as what had happened in Bophal tragedy.

4.5 Modification Cost Evaluation

The modification cost will includes equipment purchasing cost, raw material cost as well as the utilities cost.

The cost for the modification was tabulated in Table 12 and Table 13 as shown below.

Table 12: Raw Material Cost

Route	Raw Material	Cost per lb (US $)	Flow rate(t/y)	Cost(US$/y)
C3	C3	0.51	43684	44557680
	CH4O	0.96	21353	40997760
			TOTAL	85555440
TBA	TBA	0.67	102853	137823020
	CH4O	0.96	19234	36929280
			TOTAL	174752300
iC4	iC4	0.32	154524	98895360
	CH4O	0.96	21353	40997760
			TOTAL	139893120

*List of price taken from http://www.icis.com/chemicals/channel-info-chemicals-a-z/

In considering the raw material cost, methanol is also included for each process route as it is required for esterification process. Based on Table 12, the cost of C3 route is the lowest among the three routes which cost $85555440/y. Whereas, TBA route has the highest raw material cost which is $174752300/y. Nevertheless, Lawrence cost estimation proves that iC4 has the highest raw material cost followed by TBA and C3. From Table 13, the cost of iC4 is the highest among other raw material is because of the large inventory used in the process. A large inventory may also be costly besides less safe to operate as discussed previously.

Table 13: Equipment Purchasing Cost

Route	Reactor	Distillation Colum	Storage Tank	Total Cost (US$)
C3	4	1	1	**554100**
TBA	3	1	2	**976000**
iC4	3	1	2	**1163600**

*list of price taken from http://www.matche.com/equipcost/EquipmentIndex.html

The price of equipment is vary according to the size and material used and the detail calculation is shown in the appendix. The equipment purchasing costs were estimated based on the database provided by consultant company for year 2014 retrieved from http://www.matche.com/equipcost/EquipmentIndex.html. Therefore, cost index calculation as in Peter and Timmerhaus was not used in this project.

Table 13 shows the total cost of purchasing equipment for each route. Only major equipment is considered in this evaluation. The cheapest equipment purchasing cost is C3 route followed by TBA and iC4 route.

Table 14: Cost estimation for MMA routes in US ($)

Route	Raw material cost($/y)	Equipment purchasing cost($)	No.of step
C3	85555440	554100	4
TBA	174752300	976000	3
iC4	139893120	1163600	3

It is clearly shown that the number of process step does not affect both raw material and equipment purchasing cost at all. The difference in raw material cost is due to the difference in inventories of each process route whereas the difference in equipment purchasing cost is related to the specification of the equipment used. TBA route has the highest raw material cost followed by iC4 and C3 route as it has high raw material inventory. Meanwhile for equipment purchasing cost, iC4 is the most expensive route followed by TBA and C3. This is due to the elimination of equipment in storage step for iC4 route. Referring to the cost estimation done by Lawrence, C3 has the least cost of purchasing equipment followed by TBA and iC4. The differences may due to the time factor which affects the prices.

4.6 Relating Inherent Safety to Cost

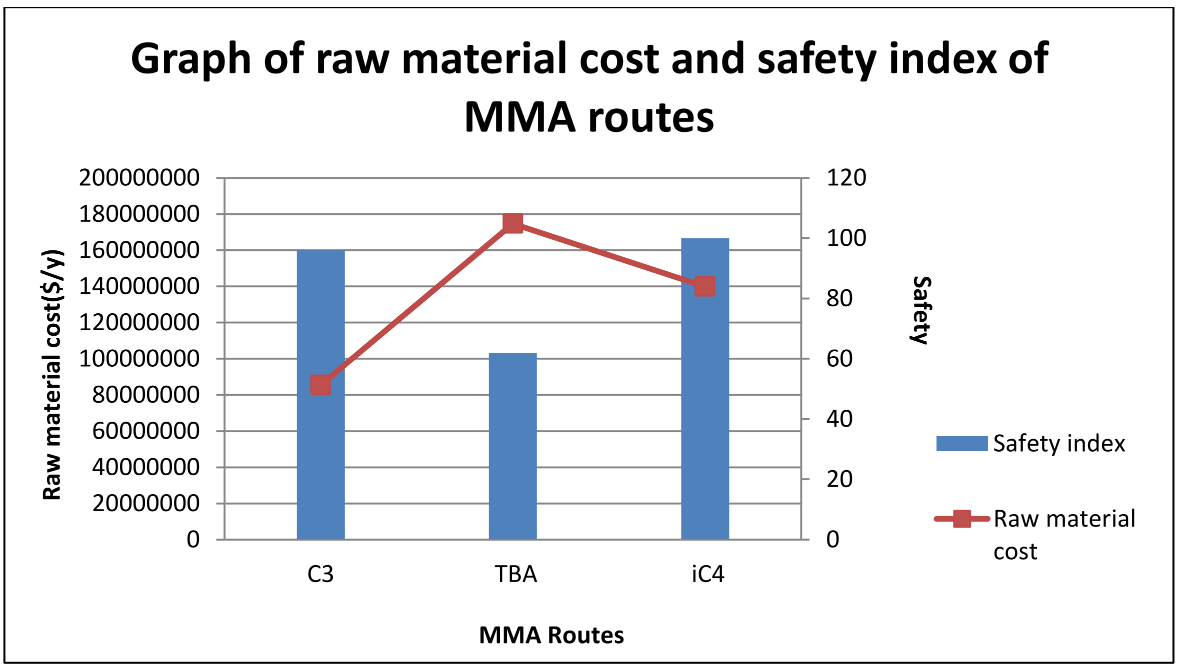


Figure 7: Graph of raw material cost and safety index of MMA routes

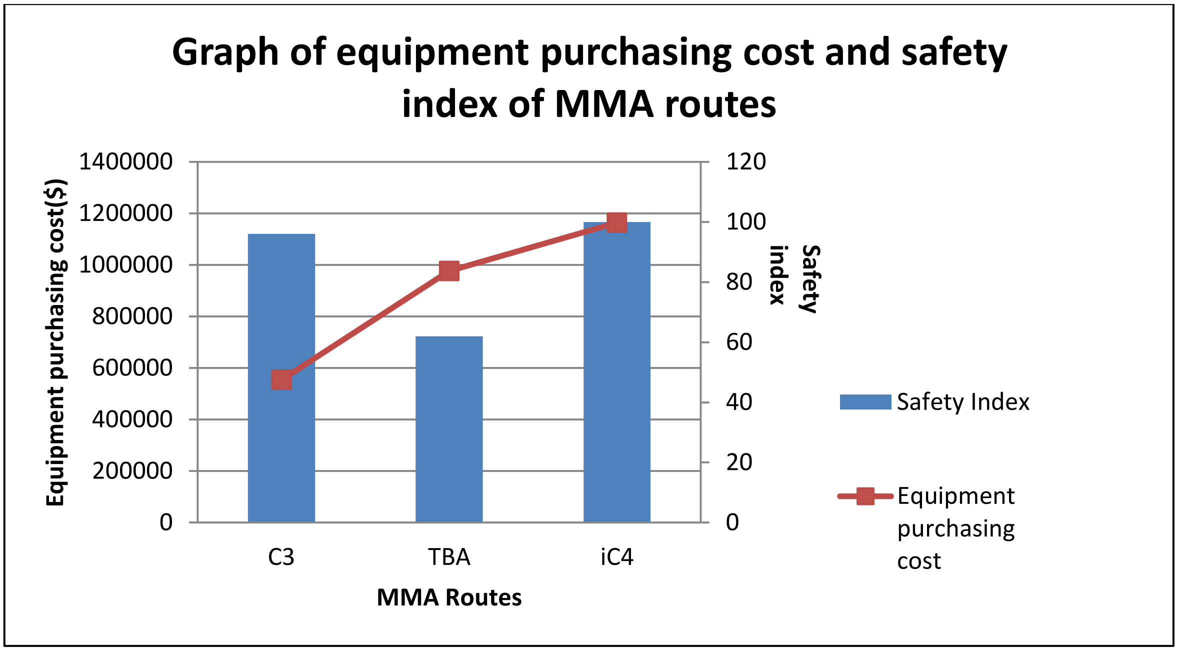


Figure 8: Graph of equipment purchasing cost and safety index of MMA routes

Figure 7 and Figure 8 compares the raw material cost and equipment purchasing cost with the inherent safety of the route respectively. C3 route is the cheapest route comparing its raw material cost and equipment purchasing cost with second highest safety index. Whereas TBA based route has the lowest safety index which is the safest route. Nevertheless, it has the highest raw material cost and moderate cost of purchased equipment. iC4 has the highest safety index which is not safe with moderate amount of raw material cost and expensive cost of purchased equipment. These two graphs conclude that inherently safer design does not necessarily be the cheapest process. Nevertheless, there is much other cost that should be taken into consideration in estimating the cost in the preliminary design which may need a longer time to work on.

4.6 Problem Encountered

While conducting this project, there are few problems encountered by the author especially in terms of time constrain and lack of data. The modification cost should include raw material cost, equipment purchasing cost as well as utilities cost. However, due to the time constrain and limited data, utilities cost is not calculated. In order to calculate the utilities cost, the author need to develop process flow diagram (PFD) of each process routes. Despite that, only major equipment is considered in determining the equipment purchasing cost.

CHAPTER 5
CONCLUSION AND RECOMMENDATION

Inherent safety design implementation is very synonym in chemical industry for safety purposes. This implementation is preferably being done in the preliminary stage or design stage. This is because preliminary stage is still in the planning stage where the ISD can still be modified. Choosing the right process step which is; the safest route and economically feasible is one of the ways in implementing ISD in preliminary stage. This study has shown that the decision in choosing a right process step is very important before proceeding with other stage. In general, it can be concluded that the TBA based route is the safest alternatives in MMA production. However, the TBA based route raw material cost is the most expensive among others. Meanwhile, the amount is acceptable for equipment purchasing cost. Furthermore, inherently safer design does affect the economic feasibility of a process. Last but not least, the safest design does not necessarily be the cheapest design alternative.

While conducting this research project, the author has come out with few recommendations in order to ease the future work. First and foremost is to develop PFD and P&ID so that the cost estimation would be much more precise. PFD and P&ID provide many detail information such as the equipment used as well as the safety and control measure. Secondly is to include utilities cost and other cost in the cost evaluation. Modification cost is supposedly includes the utilities cost. However due to the lack of information, the utilities cost is not calculated. The absence of utilities cost more or less would affect the result. Last but not least, in the cost evaluation section, the author had used a link from a website to estimate the equipment cost. This cost might be varied from time to time although the cost is by 2014. Therefore, the author suggested to use both the link provided as well as the cost index as in Peter and Timmerhaus so that the calculation would be more precise.

REFERENCES

[1] K. Kidam, M. H. Hassim, and M. Hurme, "Enhancement of Inherent Safety in Chemical Industry."

[2] T. Overton and G. M. King, "Inherently Safer Technology: An Evolutionary Approach," 2006.

[3] G. Gómez, S. Rodríguez, J. Cadena, and F. Muñoz, "Kletz's legacy for developing countries: Simple systems based on inherently safer design," *Journal of Loss Prevention in the Process Industries,* vol. 25, pp. 843-847, 2012.

[4] C. R. Deddis, "Process Economics," *CHEMICAL ENGINEERING AND CHEMICAL PROCESS TECHNOLOGY,* vol. IV.

[5] *Inherently Safer Chemical Processes: A Life Cycle Approach*, 2nd Edition ed. Center for Chemical Process Safety: John Wiley & Sons 2009.

[6] D. C. Hendershot, "An Overview of Inherently Safer Design," 2006.

[7] M. S. Peters, K. D. Timmerhaus, and R. E. West, "Plant Design and Economics for Chemical Engineers," 2003.

[8] W. Idriss, G. Andotra, and D. Natarajan, "Inheret Safety," 2009.

[9] E. Broughton, "The Bhopal disaster and its aftermath: a review," *Environmental Health: A Global Access Science Source,* 2005.

[10] D. W. Edwards, "Export Inherent Safety NOT Risk."

[11] "INVESTIGATION REPORT : Pesticide Chemical Runaway Reaction Pressure Vessel Explosion," INSTITUTE WEST VIRGINIA 2008-08-I-WV, 2011.

[12] *The Use and Storage of Methyl Isocyanate (MIC) at Bayer CropScience*: The National Academies Press, 2012.

[13] J. E. S. Venart, "Flixborough: The Disaster and Its Aftermath," in *Petrochemistry Handbook*, ed.

[14] (8 April 2014). *Flixborough (Nypro UK) Explosion 1st June 1974*

Available: http://www.hse.gov.uk/comah/sragtech/caseflixboroug74.htm

[15] F. I. Khan and P. R. Amyotte, "Integrated Inherent Safety Index (I2SI) : A Tool for Inherent Safety Evaluation," 2004.

[16] M. Rahman, A.-m. Heikkila, and M. Hurme, "Comparison of Inherent Safety Indices in Process Concept Evaluation," 1996.

[17] D. Lawrence, "Quantifying Inherent Safety of Chemical Process Routes," 1996.

[18] Y. Seo, D. Chang, J.-Y. Jung, C. Huh, and S.-G. Kang, "Economic Evaluation of Ship-based CCS with Availability," *Energy Procedia*, vol. 37, pp. 2511 – 2518, 2013.

[19] C. Palaniappan, R. Srinivasan, and R. Tan, "Selection of Inherently Safer Process Routes : A Case Study," *Chemical Engineering and Processing* vol. 43, pp. 647-653, 2002.

[20] J. P. Gupta, D. C. Hendershot, and M. S. Mannan, "The Real Cost of Process Safety - A Clear Case for Inherent Safety," *Trans IChemE*, vol. 81, 2003.

[21] Index of Process Equipment [Online]. Available: http://www.matche.com/equipcost/EquipmentIndex.html

[22] Indicative Chemical Prices [Online]. Available: http://www.icis.com/chemicals/channel-info-chemicals-a-z/

[23] E. J. Bernechea and J. Arnaldos, "Optimizing the design of storage facilities through the application of ISD and QRA," *Process Safety and Environmental Protection*, 2013.

[24] E. J. Bernechea and J. Arnaldos Viger, "Design optimization of hazardous substance storage facilities to minimize project risk," *Safety science*, vol. 51, pp. 49-62, 2013.

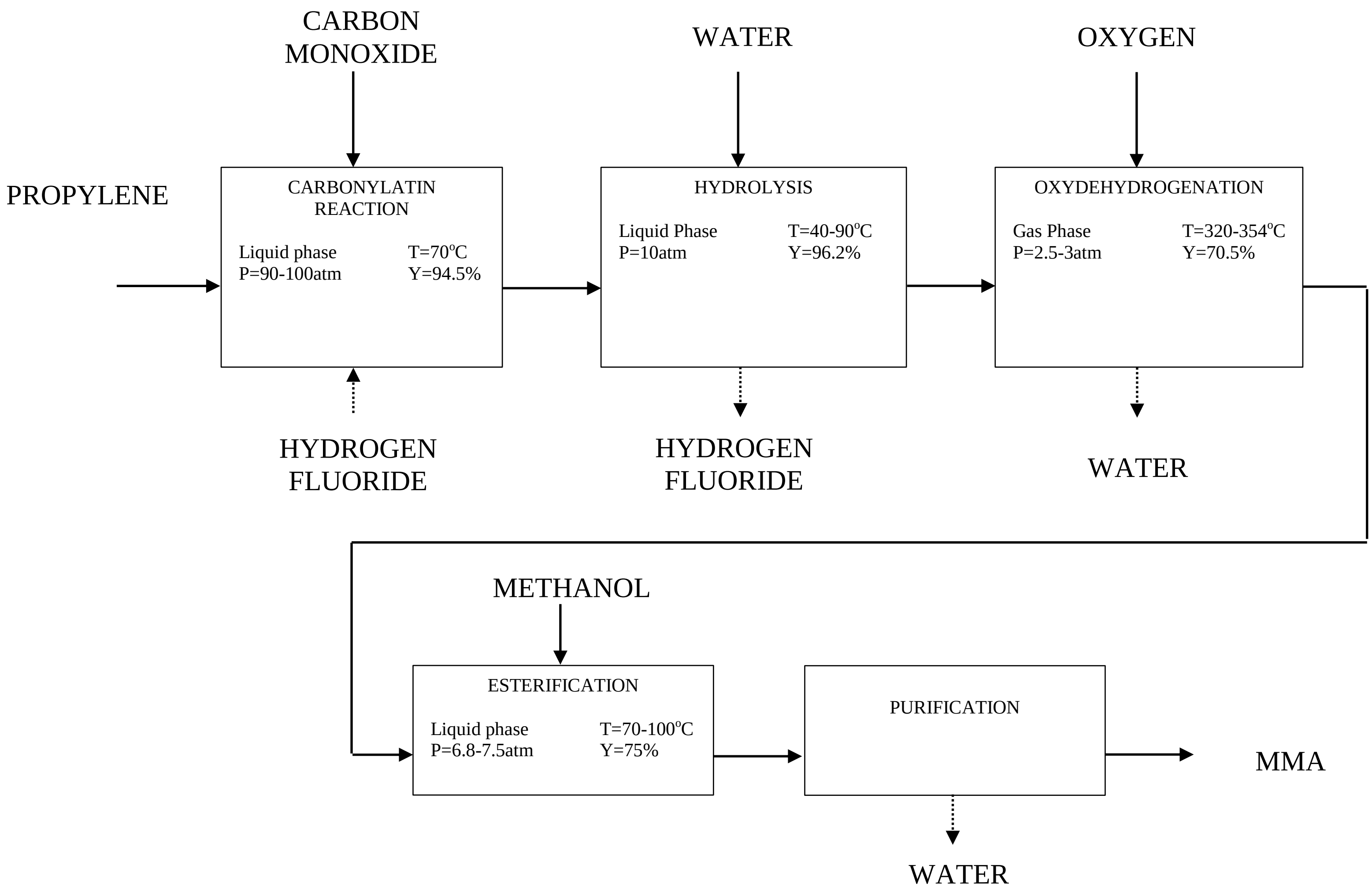
[25] A. I. Chatzimouratidis and P. A. Pilavachi, "Technological, economic and sustainability evaluation of power plants using the Analytic Hierarchy Process," *Energy Policy*, vol. 37, pp. 778-787, 2009.

[26] H. Medina, J. Arnaldos, and J. Casal, "Process design optimization and risk analysis," *Journal of loss prevention in the process industries*, vol. 22, pp. 566-573, 2009.

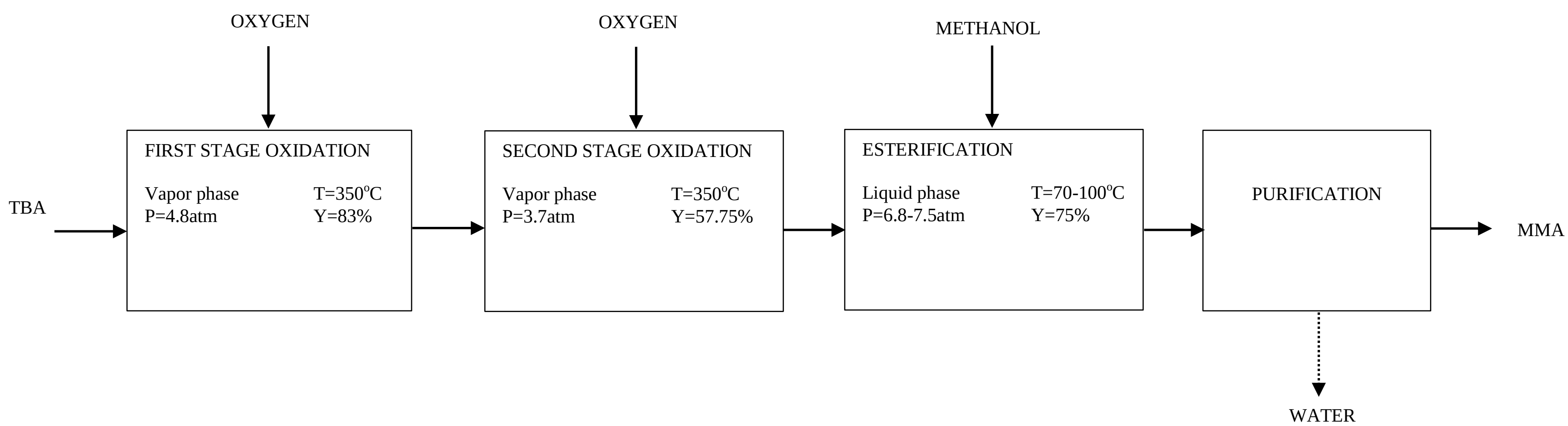
[27] D. Mignard, "Correlating the chemical engineering plant cost index with macro-economic indicators," *Chemical Engineering Research and Design*, vol. 92, pp. 285-294, 2014.

APPENDICES

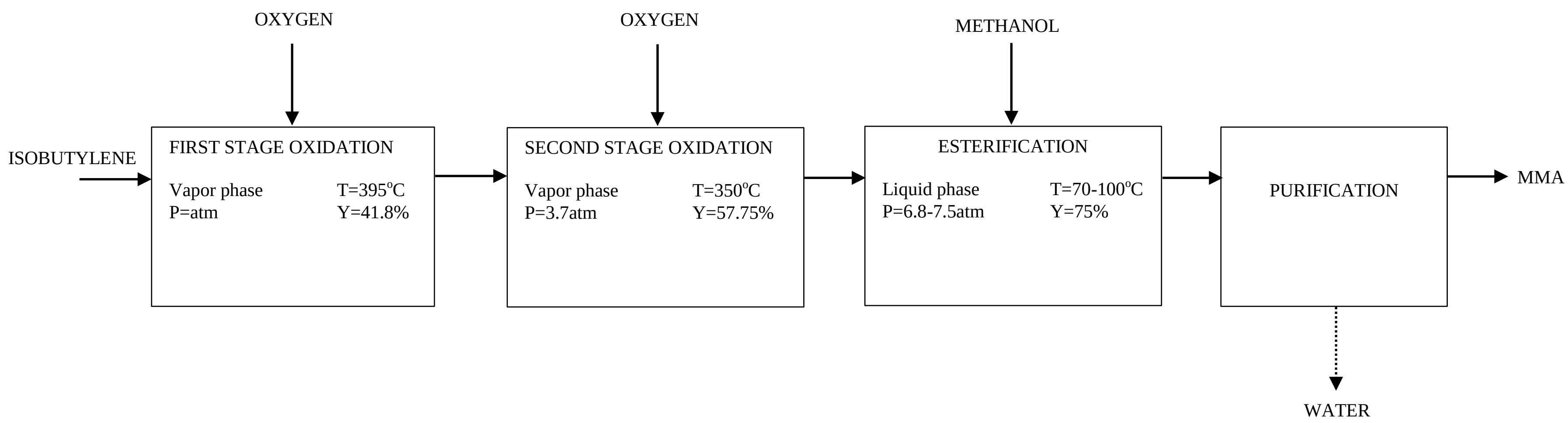
APPENDIX A – PROPYLENE BASED ROUTE DIAGRAM



APPENDIX B - TBA BASED ROUTE DIAGRAM



APPENDIX C – i-C4 BASED ROUTE DIAGRAM



APPENDIX D – DETAIL OF EQUIPMENT PURCHASING COST

Route	Equipment	Type	Size	Material	Cost
C3	Reactor	Jacketed, non agitated	3200gal	Carbon Steel	27400
		Jacketed, non agitated	3500gal	Carbon Steel	29200
		Jacketed, non agitated	3300 gal	Carbon Steel	20300
		Jacketed, non agitated	2600 gal	Carbon Steel	23500
	Distillation Column	Column	22000 lb	Carbon Steel	103900
	Storage tank	Vertical, Cone roof, Flat bottom	739000 gal	Carbon Steel & API	349800
				Total	**554100**
TBA	Reactor	Jacketed, non agitated	5000 gal	Carbon Steel	37900
		Jacketed, non agitated	3000 gal	Carbon Steel	26100
		Jacketed, non agitated	2500 gal	Carbon Steel	22800
	Distillation Column	Column	20000 lb	Carbon Steel	97700
	Storage tank	Vertical, Cone roof, Flat bottom	1141000 gal	Carbon Steel & API	463900
		Vertical, Cone roof, Flat bottom	327600 gal	Carbon Steel & API	327600
				Total	**976000**
iC4	Reactor	Jacketed, non agitated	8100 gal	Carbon Steel	54000
		Jacketed, non agitated	3300 gal	Carbon Steel	28000
		Jacketed, non agitated	2600 gal	Carbon Steel	23500
	Distillation Column	Column	22000 lb	Carbon Steel	103900
	Storage tank	Vertical, Cone roof, Flat bottom	1713900 gal	Carbon Steel & API	604400
		Vertical, Cone roof, Flat bottom	739000 gal	Carbon Steel & API	349800
				Total	**1163600**