CHAPTER 1

INTRODUCTION

1.1   Problem statement

In the chemical plants, especially, multipurpose and multiproduct plants, processes are modified and developed quite frequently to release a new or customized product or to meet the demand of the product in the competitive market. So, safety, health and environment assessment is very important in order to fulfill the safety, environment and health regulations and economic practical so that the process developments are excellent. Moreover, to consider these key-factors in early stages of chemical process design can make processes profitable, environment and health friendly, safe and competitive by reducing redesign or reimplementation costs.

The concept of integrated process development (Hungerbühler et al., 1998) stresses the importance of considering all economic as well as environmental, health and safety aspects starting from the early stages of developing a new chemical process. Thus, to fulfil all these aspects, various methods were developed to make the design feasible, less hazardous, environment and health friendly. Each method has its particular characteristics and is suitable for assessing some selected aspects or purposes.

The old methods consider the environment issue after designing it. So, most of the design will add on treatment facilities in order to treat all the waste and effluent that are discharged. This will cost more to the plant on the operation and maintenance.

Nowadays, many of the design frameworks take into consideration the environmental factor in the preliminary design stages but different technique and approach. Life Cycle Assessment (LCA) for example, is a technique for assessing the environmental aspects and potential impacts associated with a product (SFS-ISO 14040). Though the approach of LCA excellently integrates many aspects of environmental protection and is in fact a helpful innovative tool in green chemistry, it also has some major weaknesses. The

method major concern is on the goal which is the product (most of chemical plant concern). In risk assessment method, the approach is more on designing a safe plant. In risk assessment steps, inherent safety method are been applied in order to control the hazard. The environment issues is been assess when the hazard has been identified.

Therefore, a study have to be done in order to improved the plant design framework where the environmental concern are been evaluate in the earlier stage while designing a plant.

1.2   Objective

The main objective for this project is to develop a methodology using inherent safety and waste minimization concept which take into consideration the environment factor in earlier design stage. This methodology will minimize effluent, waste and pollution that will be released to the environment. The other minor objectives of this project are as follows:

1. To study and to be familiar with the inherent method/concept so that it can be implement in the project
2. To identify and analyst the available methodologies that are been used in the industry at the present.
3. To determine the potential improvements for the available approaches
4. To determine the suitable analytic techniques to minimize the waste, effluent and pollution.
5. To develop a tool using the Microsoft Excel or any other spreadsheet

1.3   Scope of Study

The primary focus of the project is to develop a methodology to design a plant where the environment factor is taking into account in earlier stage (flowsheeting and designing stage). The studies also focus on applying the inherent safety concept for waste minimization and environment. Tests and analysis will be conducted using HYSYS simulation to approve that the framework can be implemented. The simulation will be test on a sample refinery plant design. All the calculations involved will be organized and programmed in Microsoft Excel or any other spreadsheet software. Meanwhile, further research and development would be continuously practiced to ensure satisfactory results are achieved. The project is assigned to be completed within two semester's time.

CHAPTER 2

LITERATURE REVIEW

2.1 Environmental Issue

The amount of solid waste generated in Malaysia increased from 16200 ton/day in 2001 to 19000 ton/day in 2005 (Malaysia, 2006). Based on a research by Nasir et. al (1998), they estimated that wastes generation increased 4% annually. Thus, it is estimated that the industrial solid waste generation has increased from 7721.58 ton/day in 1994 to 11519.24 ton/day in 2005. But the hazardous waste generation varied in the period of 1994 to 2005. The trend below shows the waste generation in Malaysia
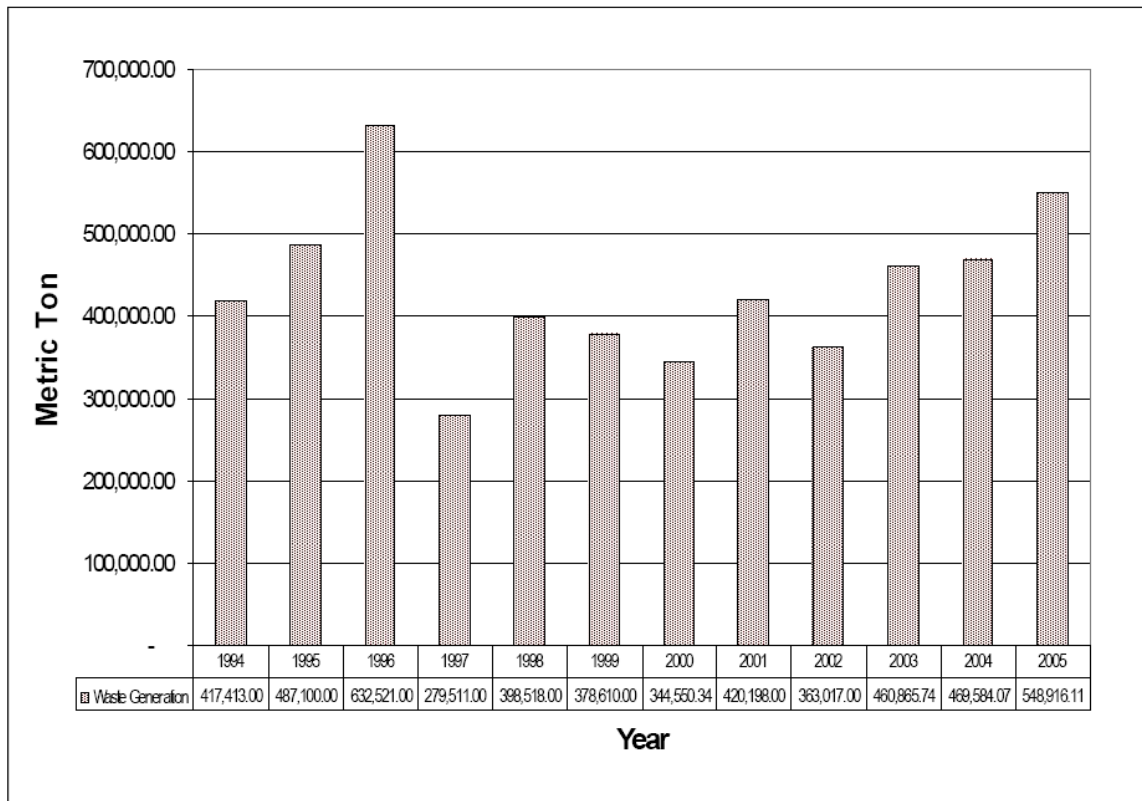

Figure 2.1: Toxic and hazardous waste generation in Malaysia (1994 – 2005)

Nasir et. al. (1998) also found that industries in Malaysia contribute 30% of solid wastes. So in this research, the author uses the inherent environmental protection analysis method to minimize the waste produce in the process. By doing this, the environmental issue can be reduce while in the preliminary design stage.

2.2   Types of environmental pollutants and waste

2.2.1   Effluent

The definition of effluent is generally considered to be water pollution, such as the outflow from a sewage treatment facility or the wastewater discharge from industrial facilities (http://www.absoluteastronomy.com/topics/Effluent). In this project, the author classes the effluent type into two which are chemical effluent (undesired product) and wastewater.

2.2.2   Waste

Industrial waste is a type of waste in term of material and substance produced by industrial activity, such as that of factories, mills and mines. Industrial waste can be in the form of liquid or solid (http://en.wikipedia.org/wiki/Industrial_waste). But then, in this project waste will be considered as a solid phase. Most of the industrial wastes are hazardous and toxic.

2.2.3   Air Pollution

The definition of air pollution is the presence in the atmosphere of one or more contaminants in such quality and for such duration as is injurious, or tends to be injurious, to human health or welfare, animal or plant life. It is the contamination of air by the discharge of harmful substances. There are many negative impacts by the air pollution such as it can cause health problem and also damage the environment property. (http://www.megaessays.com/viewpaper/19048.html)

2.3   Available Plant Design Methodology and Consideration

2.3.1   Risk Assessment Method

There are two major studies in risk assessment method which includes (Daniel A.C and Joseph F. L, 2002):

1. Incident identification

   - Describes how an accident occurs.

   - Frequently includes an analysis of the probabilities.

2. Consequence analysis

   - Describes the expected damage.

   - Includes loss of life, damage to the environment or capital equipment and day's outage.

In many plant designs, the designers always use the general risk assessment method to identify the possible risk that might happen in the plant. In the risk assessment method, (National Occupational Health and Safety Commission Report, 1995) generally include the following steps:

1. Identifying hazard
2. Assessing the risk
3. Controlling the hazard
4. Review

In risk assessment method, the inherent safety approach has been applied in controlling the hazard. Risk assessment is more on eliminated and reduced the hazard material in order to have a safe plant design.

Nowadays, there are many integrated risk assessment that have been developed. The risk assessments are more details and the scopes are smaller. One of the examples is the environment risk assessment where the environment issues as the major concern. These underlying principles are developed from those laid down by Covello and Merkhofer (Covello and Merkhofer, 1993).

Environment Risk Assessment (ERA) includes a number of steps:

- Problem Formulation
- Hazard Identification
- Release Assessment
- Exposure Assessment
- Consequence Assessment
- Risk Estimation

Based on the steps, ERA is more specific in the environment. The environmental aspect will be determined quantitatively and qualitatively. The environment risk assessment also did not taken as a whole in minimizing the waste, effluent and pollution in the approach. Again ERA has the same approach with the risk assessment method where the main objective is to have a safe plant design.

2.3.2   Life Cycle Assessment

Life Cycle Assessment (LCA) is a method of assessing the environmental impacts of products and services. The total environmental impact is assessed by calculating resource consumption and substances released considering the entire product life cycle, including not only the production and manufacturing of base materials, beginning with the extraction of resources, when creating a product, but also the product use and end-of-life disposal stage.(http://www.aist.go.jp/aist_e/annual/ 2006/environment/lca_center/lca_center_main.html).

In this method, the assessment is on the chain of materials and energy in the life cycle of the product. The environmental effect also has been considered. LCA has been established in international standards (ISO-14040~43) as a method of assessing the environment-friendliness of products and is already widely used by many companies and other organizations.

According to the ISO 14040 (Thomas J.A.G, 1977) and 14044 (Gilliland M.W and A. Bendavid-Val, 1978) standards, a Life Cycle Assessment is carried out in four distinct phases.

1. Goal and scope
2. Life cycle inventory
3. Life cycle impact assessment
4. Interpretation

Based on the step above, the major concern of the study will be the goal and the scope. In most of the chemical process plant, the goal is the product. Thus, the assessments have been made to fulfill all the requirement (safety, environment issue, economic and health) based on the product obtained. In this approaches, it focuses on the overall impact of the production, use and disposal of products rather than analysis it locally (Cheremisinoff N.P, 2001). The outputs (in the form of air emissions, water emissions or solid waste) of the process are being assess so that the environment impact does not violent the environment law.

2.3.3 SREST-Layer-Assessment method

This method can be used efficiently and quickly in laboratory where substance data and reaction recipe is defined and in conceptual flow-sheet stage where a rough sketch of flow-sheet is prepared with the list of major unit-operations involved (Shailesh Shah et al, 2005). The method can help chemists and chemical engineers in conducting the following steps:

1. To collect the property data (for example, environmental, toxicity, physical and chemical properties).
2. To assess the substances for environmental, health and safety aspects with the help of collected property data.
3. To acquire reactivity/incompatibility information from databases.
4. To predict reactivity/incompatibility with the help of incompatibility charts.

5. To identify different worst-case scenarios in major unit-operations.

6. To evaluate these possible worst-case scenarios.

7. To predict and recommend safety technologies to prevent and protect the plant.

8. Finally to use inherent safety principles for selecting optimal process design, reaction routes and process conditions.

There are four layers in SREST analysis. Below are the details on each layer:

1. Substance assessment layer (SAL)

   - In this layer, a list of all substance present in the process are been compiled

   - The physical and chemical properties, toxicity, environmental and safety data of the substance are collected

   - The substance then will be assessed in 11 effect categories which are mobility, fire/explosion, reaction/decomposition, acute toxicity, chronic toxicity, irritation, air mediated effects, water mediated effects, solid waste, accumulation and degradation (Koller et al, 2000).

   - The substance index for each category and the acceptable limit is used to select the material or optimize the mass used in the chemical process
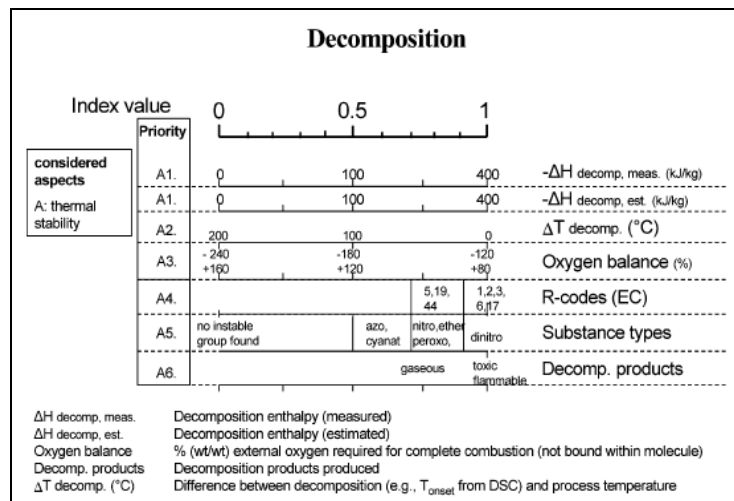

Figure 2.2: Representation of decomposition category in substance layer

2. Reactivity assessment layer (RAL)

- All the substance that possibly can come into contact are crosschecked for the reactivity with air, water, heating/cooling media, material of construction, trace impurities and with all the other substance

- The reactivity assessment is divided into 2 categories (intended reaction and unintended reaction)

- Interaction matrix will be generated to indices so that decision can be made (planning adequate material handling, pipe and instrumentation system and selecting substance) according to index result and acceptable limit.

3. Equipment assessment layer (EAL)

- In this layer, the possible worst-case scenarios related with equipment units are identified and characterized by using unit-operation model

- At present this layer covers the assessment of 4 major equipments (reactor, storage tank, distillation column and dryer)

4. Safety-technology assessment layer (STAL)

- Basically in this layer, the risk and hazard is being determined. The emissions that contribute to environmental issue is also been considered.

- If the plant and its emissions are not completely inherent safe, safety or end pipe technologies are needed to control the hazard and reduce the risk

- The selection of safety technologies around the equipments is considered as a function of results available from the other 3 layers (SAL, RAL and EAL)

So based on the layers details, the SREST layer assessment is too detailed and take time as the user needs to follow the hierarchy. On top of that, the environmental

part is just like ERA where the emission will be evaluate where the risk exist or the plant is not safe enough.
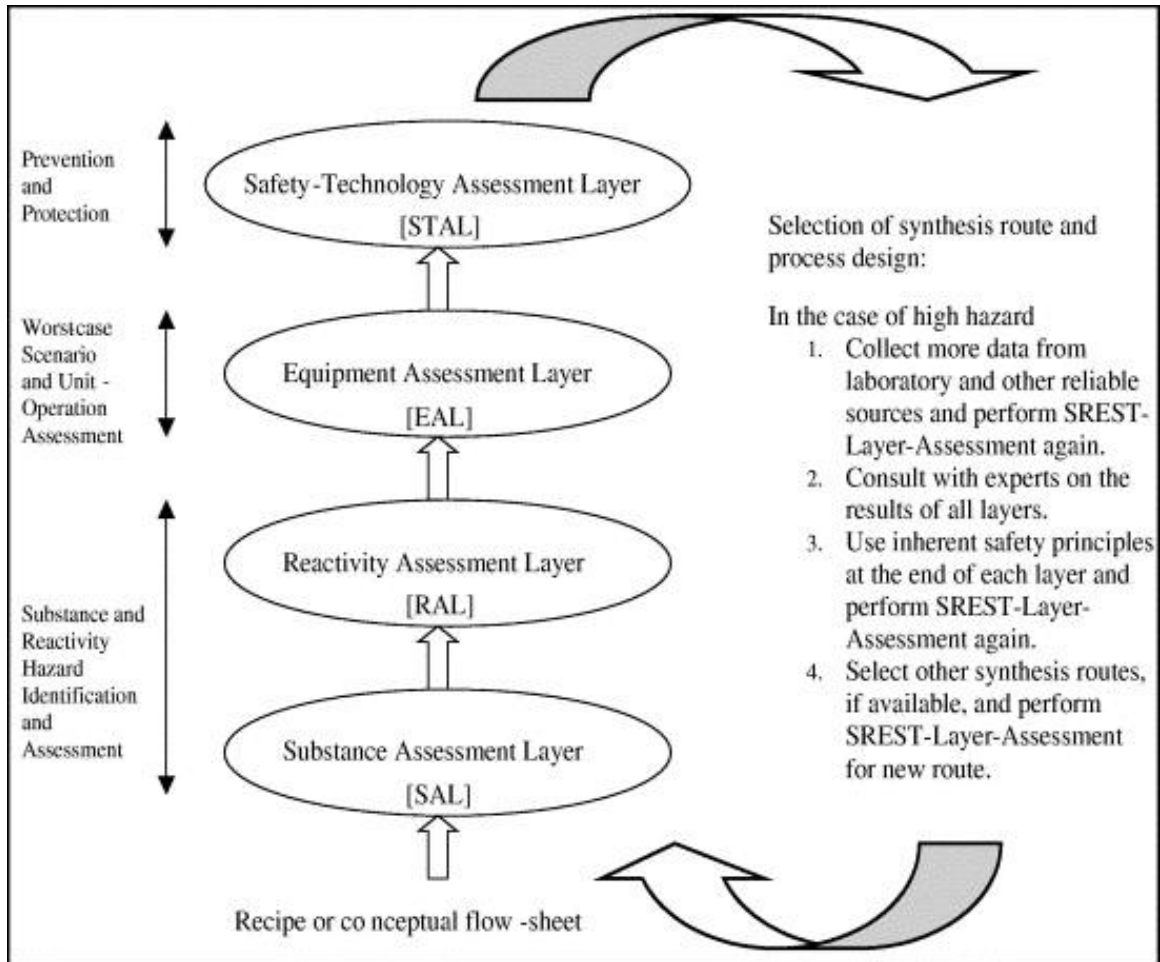

Figure 2.3: SREST-layer-assessment method with use of inherent-safety-principles.

2.4 Method used for in Inherent Environmental Protection Analysis

2.4.1 Common waste minimization method

There are 3 major methods that are commonly been used which is (Florida Atlantic University, 2002):

1. Source reduction

   ➢ This method includes process modification, chemical substitution, and improved operating procedures.

2. Recycling

   ➢ Recycling is when a waste material is used for another purpose, treated and reused in the same process or reclaimed for another process.

3. Treatment

   ➢ Treatment is where the waste will be neutralized or detoxified. These steps either decrease or eliminate toxicity or help to reduce the volume of waste.

2.4.2   Inherent safety concept

Inherent safety approaches is prevention to chemical accident. It differs from secondary accident prevention and accident mitigation as inherent safety concept relies on the development and use of technologies that prevent the possibility of a chemical accident. (N.A Ashford and G. Zwetsloot, 2002).

The principles defining inherent safety as shown in Table 2.2 were formalized by Kletz, (1991). These principles aim to reduce or eliminate hazards by modifying the design (using different chemicals, hardware, controls, and operating conditions) of the plant itself.

In terms of making plants more user-friendly Kletz also added the following:

- Avoiding Knock-on Effects
- Making Incorrect Assembly Impossible
- Making Status Clear
- Ease of Control
- Software and management procedures

Table 2.1: General principles of inherent safety (C.T. Leong and A. Mohd Shariff, 2007)

Principles	Definition
Intensification	Reduction of the inventories of hazardous materials
Substitution	Change of hazardous chemicals substances by less hazardous chemicals
Attenuation	Reduction of the volumes of hazardous materials required in the process. Reduction of operation hazards by changing the processing conditions to lower temperatures, pressures or flows
Limitation of effects	The facilities must be designed in order to minimize effects of hazardous chemicals or energies releases
Simplification	Avoidance of complexities such as multi-product or multi-unit operations, or congested pipe or unit settings
Error tolerance	Making equipment robust, processes that can bear upsets, reactors able to withstand unwanted reactions, etc.

2.5   Inherent Environmental Protection Analysis Method

The Inherent Environmental Protection Analysis (IEPA) method covered both waste minimization and inherent safety approaches. There are 4 approaches in IEPA. The approaches are as follows:

1. Substitution – replacing one material with another less hazard toxic
2. Minimization – reduce the amount of hazardous material used in the process
3. Moderation – reduce the strength of effect by moderate the parameters
4. Limit effects – end of pipe treatment

In inherent environmental protection method, the author combined both methods (waste minimization plan method and inherent safety method) in order to minimize the pollutants. This inherent environmental protection method will be as guidance for the design engineers to have a sustainable environmental design.

2.6   Differentiation between all methods

Table 2.2: Differentiation between all methods

	ERA	LCA	SREST	IEPA
Goal	To identify the hazard and the release scenario and analyze the effects/ consequences.	To assess the environmental impact through the lifecycle of product systems	To show the degree of non-ideality of chemical process with regard to SHE	To minimize the waste, effluent and pollution in the earlier design stage
Principle	Use risk assessment principle	Emerging method of risk assessment	Principles used: • Inherent Safety • Hierarchy approach	Use 2 principles: • Inherent Safety • Waste minimization
Approaches	Steps in ERA: • Problem Formulation • Hazard Identification • Release Assessment • Exposure Assessment • Consequence Assessment • Risk Estimation	Stages in LCA: 1. Goal and scope 2. Life cycle inventory 3. Life cycle impact assessment 4. Interpretation	Has 4 layer: 1. SAL 2. RAL 3. EAL 4. STAL	Has 4 approaches: 1.Substitution 2.Minimization 3.Moderation 4.Limit of effects

From the table above, it clearly seems that each method differs to each other. And for ERA and LCA, the principle is the same using the risk assessment principle.

2.7   Pollution prevention and waste minimization benefits

Most of the plants and refineries that implement pollution prevention and waste minimization program experienced many benefits. It is not only the environmental benefits but also the cost benefits. Below are some of the benefits based on U.S EPA (www.epa.gov/wastes/nonhaz/industrial/guide/pdf/chap3)

1. Protecting human health and environment
    ➢ By decreasing the volume or toxicity of process materials and wastes reduce worker exposure to potentially harmful constituents. Moreover, it also preventing the release and disposal to the environment. It which also reduce human and wildlife exposure and habitat degradation.

2. Saving money in cost
    ➢ Pollution prevention activities help the industrial processes and equipment more resource-efficient. This will increased the efficiency production, saves raw material, labor cost and maintenance cost. Besides, it is also can saved the money on the waste disposal cost

3. Simpler design and operating conditions
    ➢ By reducing the risks associated with waste can allow wastes to be managed under less stringent design and operating condition.

4. Improved work safety
    ➢ Less toxic and less physically dangerous materials in processing can improve worker safety by reducing work-related injuries and illness.

5. Higher product quality
    ➢ Having waste in the product in some operation sometimes will fail the quality inspection. So by minimizing waste in those cases is inextricably linked with process changes that improve quality

6. Building community relations

> Implementing a pollution prevention program, make people aware of it. Environmental protection and economic growth can be compatible objectives. Additionally, conversation and discussion among all parties in the development of pollution prevention plans can help identify and address concerns

CHAPTER 3

THEORY

Inherent Environmental Protection Analysis Theory

Below are the details on the IEPA approaches theory. In this part there are four major components which are substitution minimization, moderation and limits of effect

3.1 Substitution

In substitution, the approach is a combined concept of inherent safety and waste minimization concept (source reduction). User will replace one material with another of less hazard/toxic. Based on a research by EHS Florida Atlantic University in 2002, the hazardous wastes generation can be minimize and eliminate by changing the processes and practices (or also referred as source reduction). Source reduction methods include process modification, chemical substitution and improved operating procedure.

There are some factors that usually play role in the realization and outcome of a substitution process (F. Oosterhuis, 2006):

- The availability of the substitute (i.e. it should be developed and tested to a sufficient extent)
- Availability of information on the substitute and its consequences (including risks and uncertainties, as well as gaps in knowledge)
- Awareness in the organization of the problems related to the currently used substance, and preparedness to change
- The costs (investment and operational) of the substitute
- Environmental performance of the substitute;
- The risk of other negative (side) effects, both for the firm itself and for others (these may include indirect, cumulative and long term effects)

3.2   Moderation

Moderation approach helps the user to moderate the operating parameters in the process such as the temperature, pressure, concentration, flow rate and etc. By moderate these operating parameters, user be able to change the selectivity and improve the process to achieve the concentration limit and environmental regulation.

3.3   Minimization

In this approach, the amount of chemical used and toxic material present in the processing will be reduced in the preliminary stage. In this method, source reduction approach in waste minimization is been combined with the inherent safety principle. In minimization, the approach will help the user to reduce the waste in many aspect whether the leaks, spill, amount used or production of the waste.

In this approach, for minimization of chemical used amount is based on trade-off situation. User also needs to take the minimum operating cost and check whether it meets the market demand, the company goals and the safety. So, the decision making is based on the user.

3.4   Limits Effect

In limits of effect approach, the end pipe line treatment method is used where user has to add or design the facilities to minimize the waste, effluent or pollution. This effect can be used if all of others approach cannot be implement to the design (last resort if all the approaches above can not be used for minimizing the pollutant). The choice of treatment operation depends on the quality and variability of the raw water source and the treatment objective (Droste L. Ronald, 1997)

Wastewater Treatment

In this project, the wastewater treatment is focusing on industrial wastewater treatment. It covers the mechanism and processes used to treat water that have been contaminated

during the processing to release into the environment or its reuse. Wastewater treatment can be divided into two major types which are:

1. Physical-Chemical treatment
2. Biological treatment

There are many type of physical and chemical treatment in industrial. Some of the treatment is as below:

1. Screening and sedimentation
2. Mass transfer and aeration
3. Coagulation and flocculation
4. Filtration
5. Physical-chemical treatment for dissolved constituents
6. Disinfection

3.4.1 Screening and sedimentation

Screening is a method of separating particles according to size alone (Hendricks W. David, 2006). The objective of screening is to receive a feed containing a mixture of particles and separate it into underflow (that is passed through screening) and overflow (that is rejected from screening). There are 4 types of screen which are bar screen, comminutors, fine screen and microscreen.

Sedimentation is a physical water treatment process used to settle out suspended solids in water under the influence of gravity (http://en.wikipedia.org/wiki/ Sedimentation_(water_treatment), 2nd October 2009).

3.4.2 Mass transfer and aeration

Aeration serves a number of useful purposes in water treatment. Mostly aeration removes the problem substances that generally found in groundwater.

3.4.3 Coagulation and flocculation

Coagulation is defined as 'a process that involves the formation of complex hydrous oxide to reduce the surface charge of colloidal particles' (Conley and Evers, 1968). Many natural compounds from starch to iron and aluminum salt can accomplish coagulation. Besides that, synthetic cationic, anionic and nonionic polymers are also very coagulation but the cost is much higher.

3.4.4 Filtration

Filtration is the bulwark of water treatment. Filtration is used as a preliminary treatment of raw water high suspended solid contents. It also used for polishing wastewaters particularly effluents from stabilization pond system. Medium for filtration are sand, crushed anthracite, crushed magnetite, and garnet. The medium size and the pore openings influenced the filtration. There are several different criteria for the choice of filtration which are (Maryam Noor, 2007):

- Characteristics of the liquid to be filtered
- The desired quality of filtrate and the permissible tolerance
- The quality of the mass of retained material when the object is to recover
- Installation condition
- Facilities available for washing

3.4.5 Physical-chemical treatment for dissolved constituents

The removal of dissolved constituents in a water, dissolved ions, is often a challenging problem. Flocculation, sedimentation and filtration are used to remove many dissolved components. While adsorption and ion exchange are the other alternatives that do not require other unit operation.

3.4.6 Disinfection

The term disinfection refers to the inactivation of microorganism in the water. The water is not necessarily sterilized. Disinfection is applied to wastewater effluents to reduce the risk of disease for recreational users and to minimize the contamination to downstream water.

3.4.7 Biological Wastewater Treatment

Biological wastewater treatment is primarily used to remove dissolved and colloidal organic matter in a wastewater (Droste, Ronald L. 1997). There are some factors that must be taking into consideration to maximize the benefits such as (Schultz E. Thomas, 2005):

- Understand the sources of the wastewater generated
- Analyze the typical wastewater composition
- Know the discharge requirement
- Identify the events and practices within a facility that can affect the quantity and quality of the wastewater
- Aware the pretreatment ramifications

An effective biological treatment gives many benefits. Those benefits include:

- Low capital and operating cost compared to those of chemical-oxidation process
- True destruction of organics, versus mere phase separation, such as with air stripping or carbon adsorption
- Oxidation of a wide variety of organic compounds
- Removal of reduced inorganic com pounds, such as sulfides and ammonia, and total nitrogen removal possible through de-nitrification
- Operational flexibility to handle a wide range of flows and wastewater characteristics
- Reduction of aquatic toxicity

CHAPTER 4

METHODOLOGY

4.1   Generic Framework
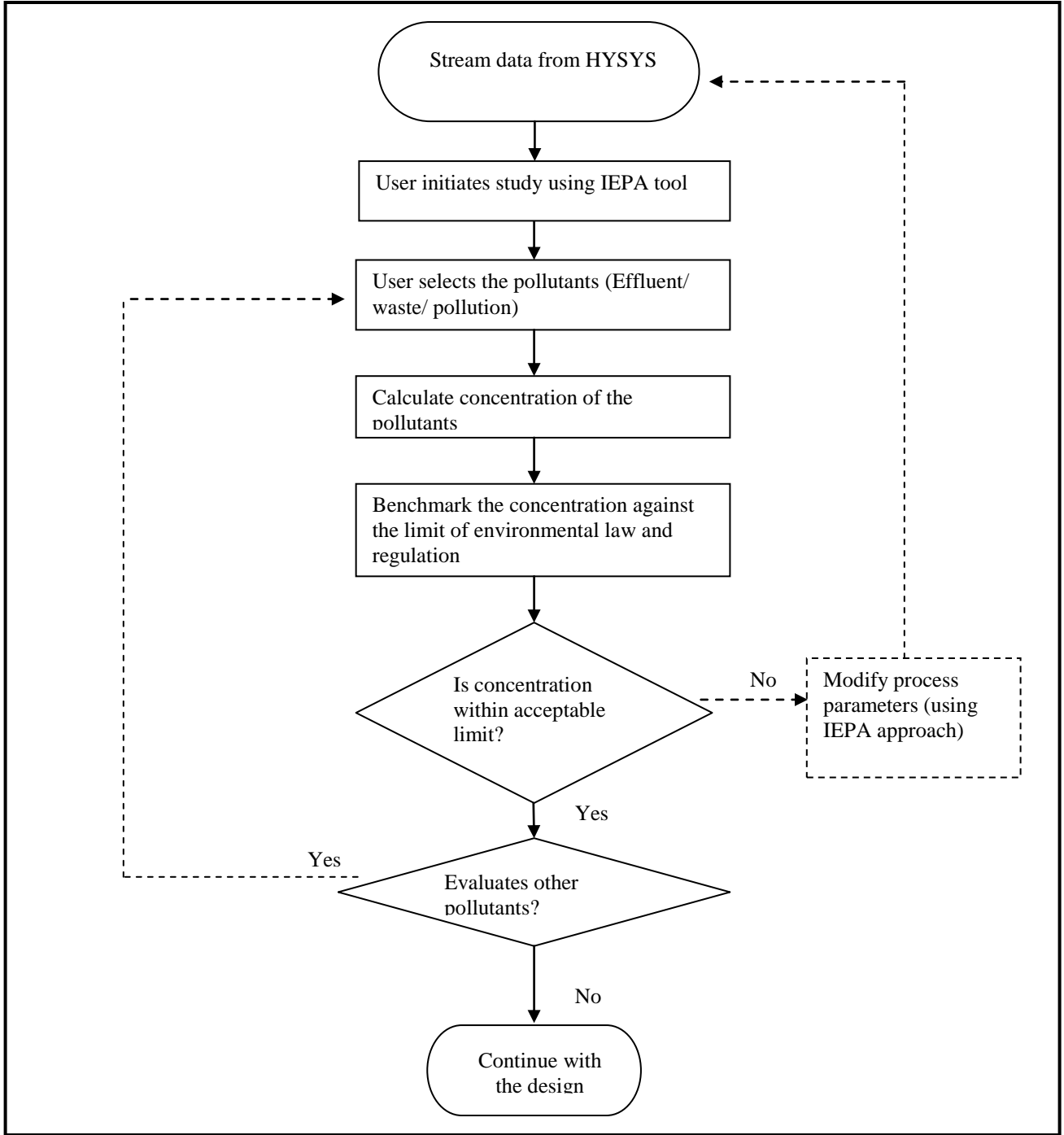
Figure 4.1: The generic framework of the IEPA tool

Figure 4.1 shows the generic framework for the overall tool algorithm. Inherent Environmental Protection Analysis (IEPA) tool is a HYSYS-Excel interface program where all the calculation will be calculated in the Microsoft Excel and the data is imported from HYSYS simulation. The design engineers can check directly the effluent, waste and pollution produced for the design in the preliminary design stage. This integrated tool will import automatically the desired data from the process simulator (HYSYS) and calculate the concentration of the pollutants. This tool also provides user the environmental report whether the process or design is acceptable or not.
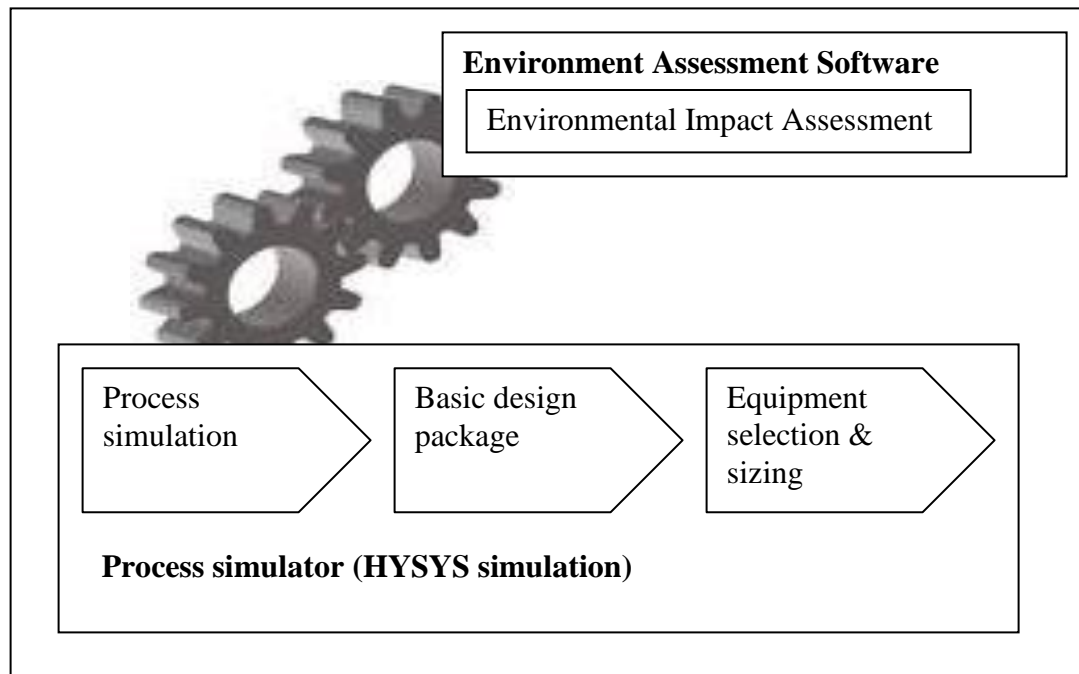
Figure 4.2: Graphical representation of the framework

4.2   General Framework details

Below are the details for the generic framework.

4.2.1   User initiates study using IEPA tool

➢ User has to initiate the study using the IEPA tool

➢ Import stream data from HYSYS simulation

4.2.2   User selects the pollutant to evaluate

  ➢ User has to choose the pollutants (waste, effluent or pollution) to be evaluated for the case study

  ➢ For each pollutant there will be divided into smaller part:

  1. Effluent – wastewater and chemical effluent
  2. Waste – toxic waste
  3. Air pollution

  ➢ User have to evaluate all the pollutants (user need to evaluate effluent, waste and air pollution) and make sure each pollutant is acceptable within the limit before continue with the design

4.2.3   Calculate the concentration of the pollutant

  ➢ The tool will calculate the pollutants concentration based in the HYSIS data stream

  ➢ From the imported stream data, user needs to choose the components to be calculated as the pollutants.

The calculation involved for each pollutant is varies with each other. There are two parts in effluent which are chemical effluent and wastewater. For chemical effluent, the pollutants will be compared in term of concentration. So the tool used simple concentration calculation to calculate the pollutants.

$$\text{Pollutant}_C = m_x * \text{mass desity (kg/L)} * 100000\text{mg}/1\text{kg} * 1\text{L}/1000\text{mL}$$

Where,

Pollutant$_C$ =   pollutant x concentration

m_x =   mole fraction for component x

- 24 -

4.2.4   Benchmark the concentration against the environmental law and
      regulation

> ➢ The calculation results will be compared to the environmental
>   regulation and indexing by Environmental Protection Agency
>   (EPA) and will provide the user the report whether the pollutants
>   are within the acceptable limit or not

4.2.5   Acceptableness

> ➢ If the result is within the acceptable limit, the user need to choose
>   other pollutants to be calculate
> ➢ If not, the user need to change the process parameters or the
>   design using inherent safety approaches to get better result

4.2.6   Modify process parameters or the design

The tool used inherent environmental protection approaches to help the user to
get the better result.

> ➢ User has to choose the inherent environmental protection
>   approaches to be used. There are 4 approaches that can be used to
>   get better result. The last choice for the user to be used is the limit
>   of effect where end pipe of treatment will be done
> ➢ After that user need to go back to the HYSYS to make any
>   changes based on the approach used

4.2.7   Calculate other parameter

> ➢ If yes, user needs to pick other pollutants until all the pollutants
>   have been evaluated. For example, user choose to evaluate
>   effluent and finished with it, then user need to proceed evaluate
>   waste until it acceptable and lastly the pollution. User need to
>   complete all pollutants before proceed with the design
> ➢ If all the pollutants have been evaluated and the results are within
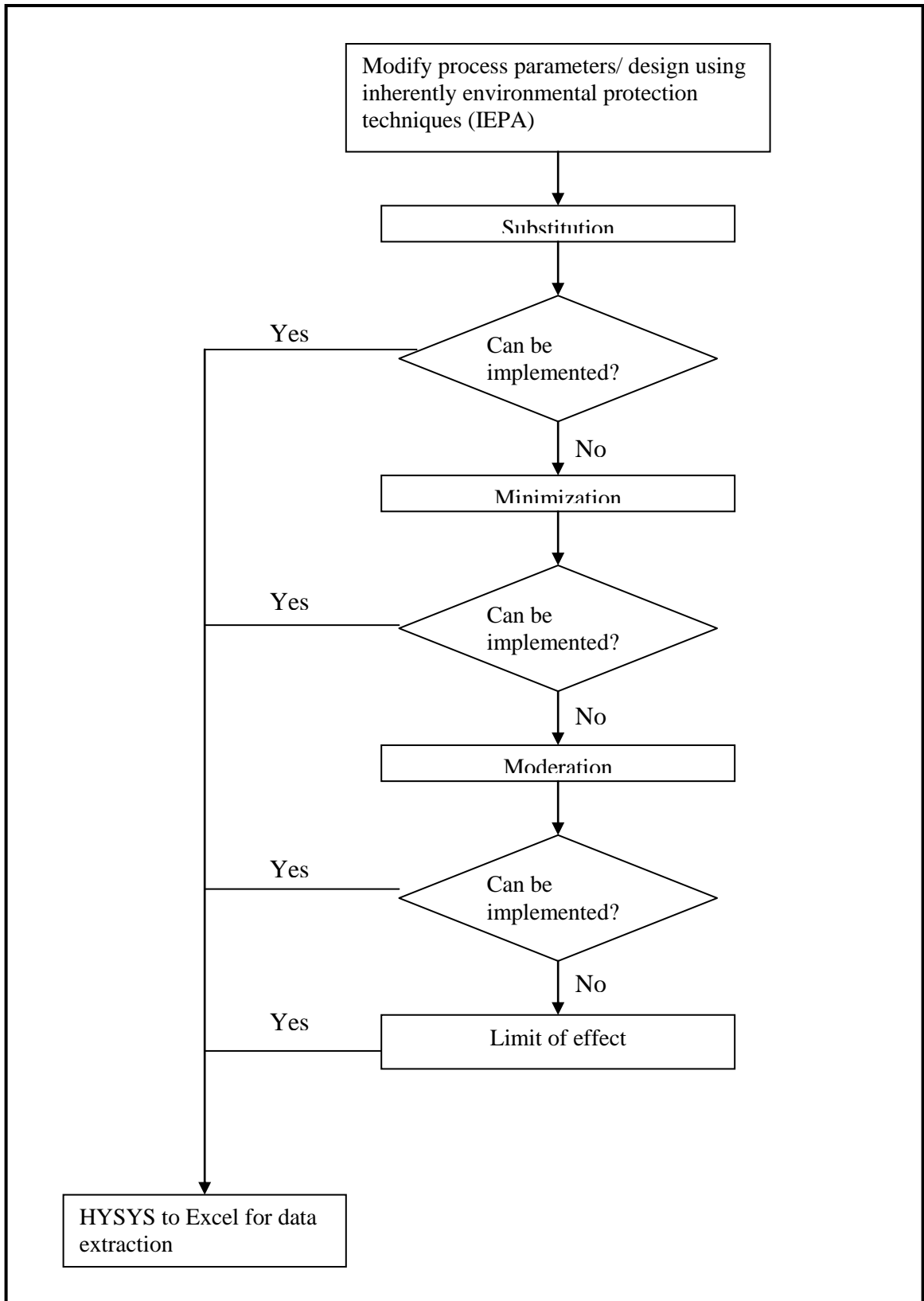>   the acceptable range, user can proceed with the design process.

Figure 4.3: The supplementary framework on modify process parameter

CHAPTER 5

TOOL DEVELOPMENTS

5.1   Tool limitations

In IEPA tool, the environmental issue to be evaluated is limits to chemical effluent only. And all the calculations for each approach is been developed based on suitability for chemical effluent. In this tool, the author also assesses the chemical effluent for reactor design.

5.2   Substitution

In this tool, the user will be provided a list of safer substitute or chemical to be used in the process. User will be provided with the details on chemical to be substitute, safer chemical and the used in the industry. So after knows the substitute chemical, user need to check the factors as in the IEPA concepts to make sure that the substitute chemical is practicable to the process

5.3   Moderation

Based on Wei Qi and M.F Malone (2009) research, the operating parameters give impact to the batch reactor distillation selectivity. Higher selectivity improved the raw material consumption where it gives lower waste production. So, in order to minimize the waste, this method will help the user to replace the strength of effect by moderate the operating parameters such as the type of reactor used and the concentration of the chemicals.

5.3.1   Parallel reaction for one reactant

General stoichiometric equation for parallel reaction using one reactant:

$A \rightarrow D$ (rate law: $k_D \, C_A^{\alpha 1}$)

$A \rightarrow U$ (raet law: $k_U \, C_A^{\alpha 2}$)

Selectivity equation

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D\,C_A^{\alpha 1}}{k_U\,C_A^{\alpha 2}}$$

So, in order to maximize the desired product, two cases must be identified.

Case 1: α1 > α2

α1 – α2 = a   where (a > 0)

So, in advance after the substitution we have:

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D\,C_A^{\,a}}{k_U}$$

To make the ratio as large as possible, we have to keep the concentration of the reactant A as high as possible during the reaction.
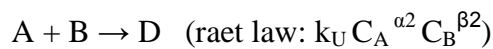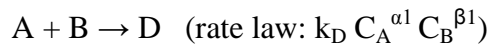
Case 2: α2 > α1

Now let α2 - α1 = b   where (b > 0)

So, in advance after the substitution we have:

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U\,C_A^{\,b}}$$

To make the ratio as large as possible, we have to keep the concentration of the reactant A as low as possible during the reaction.

5.3.2   Parallel reaction for two reactants

A + B → D   (rate law: $k_D\,C_A^{\alpha 1}\,C_B^{\beta 1}$)

A + B → D   (raet law: $k_U\,C_A^{\alpha 2}\,C_B^{\beta 2}$)

Selectivity equation

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D\,C_A^{\alpha 1}\,C_B^{\beta 1}}{k_U\,C_A^{\alpha 2}\,C_B^{\beta 2}}$$

For this type of reaction, 4 cases must be considered which are:

Case 1: α1 > α2 and β1 > β2

Let α1 - α2 = a and β1 - β2 = b,

Selectivity equation will become:

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D \, C_A{}^a \, C_B{}^b}{k_U}$$

To make the ratio as large as possible, we have to keep the concentration of the reactant A and B as high as possible during the reaction.

Case 2: α1 > α2 and β1 < β2

Let α1 - α2 = a and β2 – β1 = b,

Selectivity equation will become:

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D \, C_A{}^a}{k_U \, C_B{}^b}$$

To make the ratio as large as possible, we have to keep the concentration of the reactant A as high as possible and concentration of reactant B low during the reaction.

Case 3: α1 < α2 and β1 < β2

Let α2 – α1 = a and β2 – β1 = b,

Selectivity equation will become:

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U \, C_A{}^a \, C_B{}^b}$$

To make the ratio as large as possible, we have to keep the concentration of the reactant A and B as low as possible during the reaction.

Case 4: α1 < α2 and β1 > β2

Let α1 − α2 = a and β1 − β2 = b,

Selectivity equation will become:

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D \, C_B{}^b}{k_U \, C_A{}^a}$$

To make the ratio as large as possible, we have to keep the concentration of the reactant B as high as possible and concentration of reactant A low during the reaction

5.4 Minimization

This tool use minimizes the volume of the chemical used in order to meet the requirements and regulations. The tool also implements the element of chemical reaction engineering in this approach. Flowrate and the volume of reaction will be control in order to achieve the pollution concentration limit. The approaches and calculations are differs with the reactors type even though it base on selectivity equation. In this project, the author's scope is on batch reactor and continuous-flow reactor.

5.4.1 Batch reactor

Selectivity of reaction:

$$S_{D/U} = \frac{r_D}{r_U}$$

Batch reactor neither has inflow or outflow of reactants or products while the reaction is being carried out ($F_{jo} = F_j = 0$). If the reaction mixture is perfectly mixed, there will be no variation in the rate reaction throughout the reactor volume so the r_j can be take out from the integral.

Mole balance equation:

$$\frac{dN_A}{dt} = r_A V$$

So base on both equations, selectivity equation will become:

$$\text{Selectivity} = \frac{dN_D / dt}{dN_U / dt} \cdot \frac{1}{V}$$

Simplified the equation we get,

$$\boxed{\frac{dN_D}{dN_U} \cdot \frac{1}{V}}$$

5.4.2   Continuous-flow reactor

Selectivity of reaction:

$$\boxed{S_{D/U} = \frac{r_D}{r_U}}$$

Continuous flow reactors are almost always operated at steady state. There are three type of continuous flow reactor that is most used in industrial. But in this project, the author consider just on continuous stirred tank reactor (CSTR). CSTR is usually used for liquid phase reactions.

Design equation for CSTR

$$\boxed{V = \frac{F_{jo} - F_j}{-r_j}}$$

Where,

V = the reactor volume

F = flowrate (moles/time)

So base on the design equation, selectivity equation will become:

$$\boxed{S_{D/U} = \frac{(F_D - F_{Do})/V}{(F_U - F_{Uo})/ V}}$$

Simplified the equation above we get:

$$\boxed{S_{D/U} = \frac{(F_D - F_{Do})}{(F_U - F_{Uo})}}$$

5.5   Limit of effects

Limit of effects approach is the last alternative if other approaches cannot be implemented. In the develop tool, user will be provided with a list of treatment that is suitable to treat the chemical. The choice of treatment operation depends on the quality and variability of the raw water source and the treatment objective (Droste L. Ronald, 1997)

CHAPTER 6

RESULTS AND DICUSSIONS

6.1   Substitution

6.1.1   Case study details

The manufacturing process for traditional fiber glass insulation products utilizes a thermosetting phenol-formaldehyde based resin or binder. Glass fibers will not stick together by themselves. To hold the glass fiber together an adhesive (binder) is sprayed on the fibers. After curing in an oven, the binder holds the fibers together to keep their shape and overall form. This results in corresponding releases of ammonia, formaldehyde and phenol.

6.1.2   Results and discussion

Based on a research (State of Ohio EPA, 2002), there is other insulation product that utilizes a new acrylic binder has been introduced. The acrylic binder is used in this new fiber glass hold just like phenol-formaldehyde.

Another new product is by fusing two different types of glass together. This results in a naturally curly fiber. The glass fibers intertwine and lock themselves together. The binder is eliminated from the manufacturing process.

This recent technology also has some additional benefits. The fibers are more resilient, stronger and less prone to breakage. So, fewer fiber particles will get into air or into the installer's skin. All of these benefits will contribute to safer workplace. Moreover, the used of phenol can be minimize and reduce the releases of phenol to the environment.

6.2   Minimization

6.2.1   Case study details

In this analysis a batch reactor problem is taken. Where initially the undesired product concentration is above the concentration limit. The undesired product of this process is the phenol. Here are the results and analysis of the case study (based on H.S Fogler, 2005)
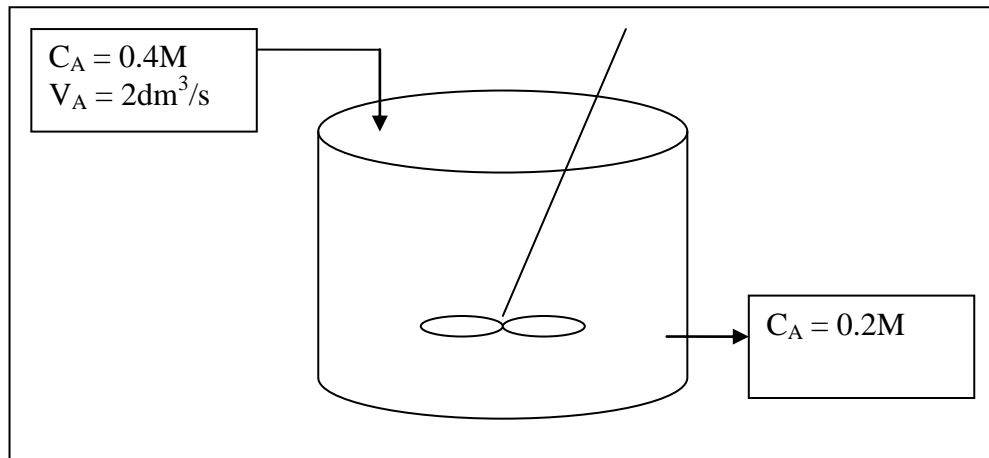

Figure 6.1: The diagram for the process

Given that a reactant A decomposes by two simultaneous reactions to form two products, one that is desired, B and undesired product Y (phenol). The concentration of A enters at 0.4M and the flow rate for the reaction is $2dm^3/s$. These reaction rate laws are as below:

$K_1C_A = 0.0015 s^{-1} C_A$

$K_2C_A^2 = 0.008\ dm^3/mol.s\ C_A^2$

6.2.2   Results and discussion

Check the concentration limit:

Component	Concentration (mg/L)	Conc. Limit (mg/L)	Report
Desired product	9152	-	OK
Undesired product	7.216	5.0	Not OK

The concentration limit report for the undesired product (phenol) is no acceptable as it exceed the limit that is given by the government. Please refer to Appendix B for more details.

This equation involved the equation of residence time for continuous stirred tank reactor.

$$V = \frac{v_0\left[C_{A0} - C_A^*\right]}{-r_A}$$

$$\tau = \frac{V}{v_0} = \frac{\left(C_{A0} - C_A^*\right)}{k_1 C_A^* + k_2 C_A^{*2}}$$

$$\tau = \frac{0.4 - 0.2}{(0.0015 \times 0.2) + (0.008 \times 0.2)}$$

Then to optimize the volume, set the mol fraction for the undesired product to the concentration limit.

$$C_Y = \frac{k_2 V}{v_0} = k_2 \tau$$

$$V = \frac{C_Y v_0}{k_2}$$

$$V = \frac{5.31E^{-5} \times 2}{0.008}$$

$$V = 0.01328 dm^3$$

After using IEPA tool, the optimum volume for the process to achieve the concentration limit is 0.01328 dm^3. The volume recommended is quite small so it depends on the user to make the decision. Please refer to the Appendix B for IEPA results.

In IEPA the decision making is depend on the user itself. User then has to calculate the total cost of the process and checked if the product can fulfill the demand in the market or not. This will be a trade-off situation.
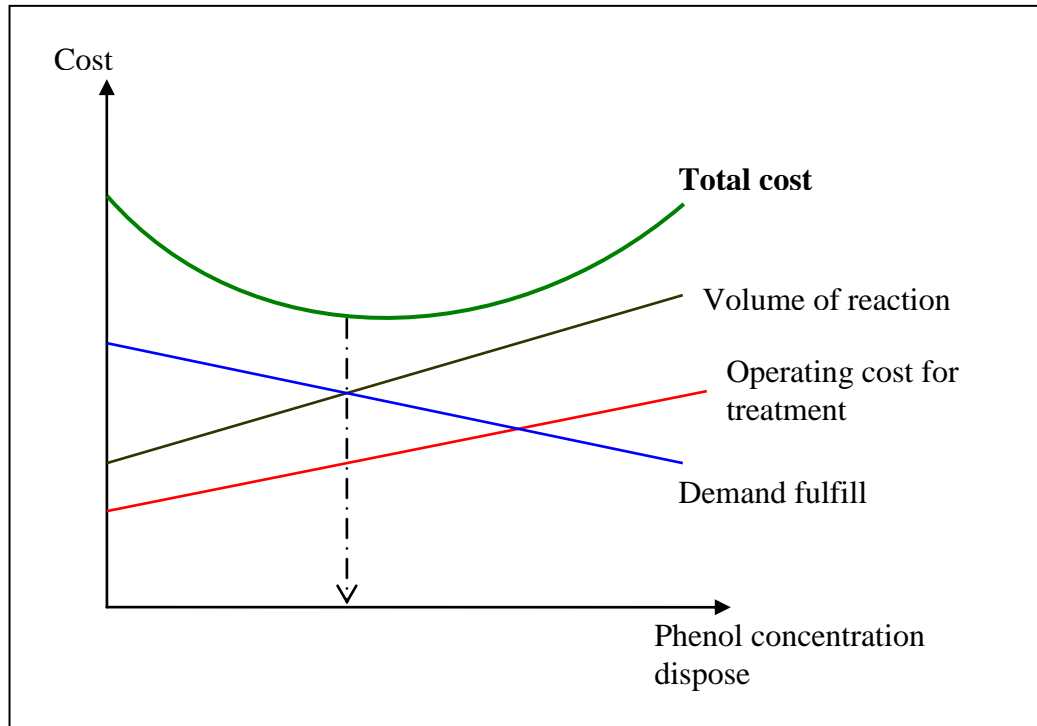
Figure 6.2: Trade-off graph that show minimum total cost

6.3 Moderation

6.3.1 Case study details

Take the same case study (as in minimization) for this case. For this approach, the important data to know is the stoichiometric equation and the rate law of the reaction. Consider that the reaction is a parallel reaction of one reactant. Below are the details on the reactions.

Stoichiometric equation:

$$A \xrightarrow{k_D} D$$
$$A \xrightarrow{k_U} U$$
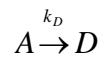
The rate law of the reaction

$$r_B = 0.0015 C_A^1$$
$$r_Y = 0.008 C_A^2$$

6.3.2 Results and discussion

Use the selectivity equation to know the efficient reactor scheme.

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D C_A^{\alpha 1}}{k_U C_A^{\alpha 2}}$$

$$\frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha 1 - \alpha 2}$$

$$\frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha}$$

Based on Elements of Chemical Reaction Engineering by H.Scott Fogler, 2006

If $\alpha 1 < \alpha 2$,

The recommendations for this reaction are as below:

- Keep the concentration of the reactant A as low as possible during the reaction

  - Diluents could be used to maintain the entering concentration of A at a low value

- A CSTR should be used because the concentration of reactant are maintained at a low level

6.4 Limits Effect

6.4.1 Case study details

Taken as the same case study for minimization and moderation, there are high concentration of phenol on the process. The phenol concentration is over the concentration limit by the government. The last approach that can be used before dispose the waste is by treating it.

6.4.2 Results and discussion

There are many techniques to treat the phenol waste stream. Below are some of the techniques that are available and be used currently.

1. VTX Oxidation Process

   Based on a research, VTX catalytic process is an efficient treatment procedure. It can treat a broad list of treatable chemicals include phenols. The VTX process does not generate noticeable sludge in water treatment applications. On top of that, VTX based treatment systems are often more efficient and provide for lower cost than other competing oxidation treatment system available nowadays (http://www.advancedoxidation.com/uploads/Industrial_Pretreatment_of_Phenol_in_Wastewater.pdf). Below are the results of the research.

   Table 6.1: characteristic of the wastewater stream

Source	Phenol mg/L	COD mg/L	pH
1	1.4	220	6.8
2	3.1	245	7.1
3	7.2	236	7.2

   Table 6.2: result after the reaction (reaction time: 3 hours)

   Wastewater Source 3

Dosage	Phenol Remaining	
	Control	VTX Treated
0.2 mls	7.0	5.5
0.4 mls	7.1	3.7
0.6 mls	7.0	2.0
0.8mls	6.9	0.6
1.0 mls	7.2	ND

2. Degradation of phenol using Anolyte

   Research by Azni Idris and Katayon Saed (2003), said that anolyte can be used for phenol treatment. They found the optimum condition which facilitates a complete degradation of phenol. Anolyte consists of reactive ions and free radicals which contribute to its oxidizing behavior. In this

research the anolyte is produced from electrochemical generation of brine solution. Below are the results from their research.
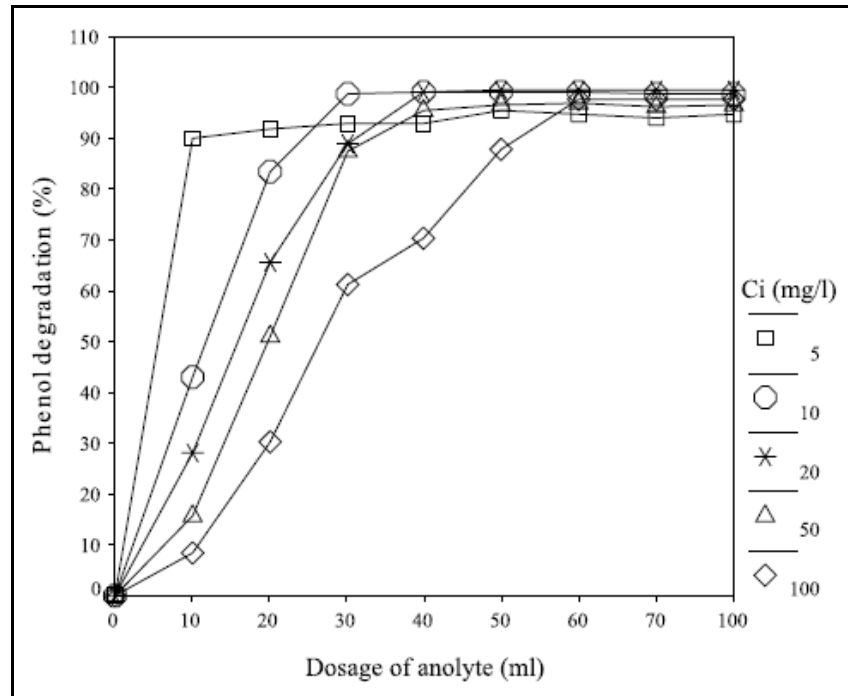

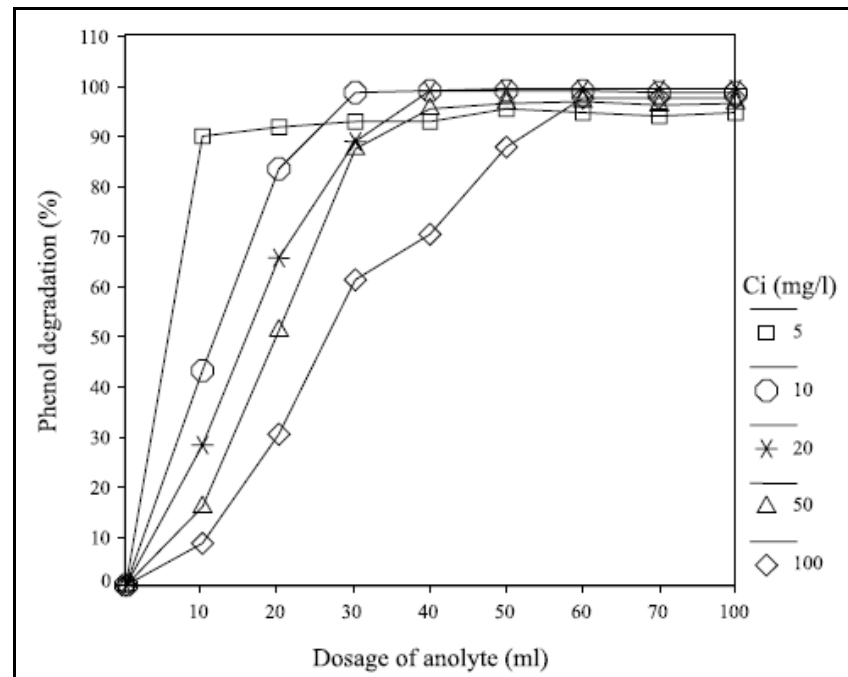Figure 6.3: Effect of anolyte dosage on phenol degradation efficiency

Figure 6.4: Effect of reaction time on phenol degradation efficiency

3. Kinetics of biological treatment of phenol wastewater in a three phase draft tube fluidized bed bioreactor containing biofilm.

The volumetric biological removal rate with biofilm is proportional to the specific surface area of the biofilm (V.Vijayagopal and P.L.Sabarathinam, 2006). The result can be shown as below.
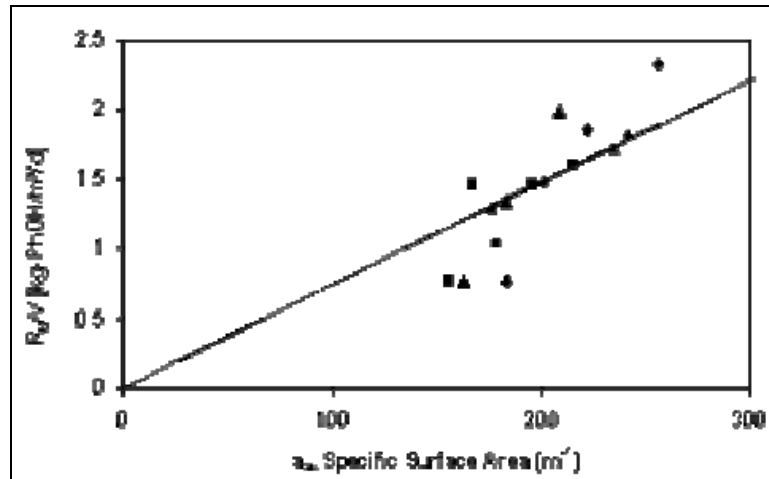
Figure 6.5: Effect of specific surface area of biofilm on phenol removal rate
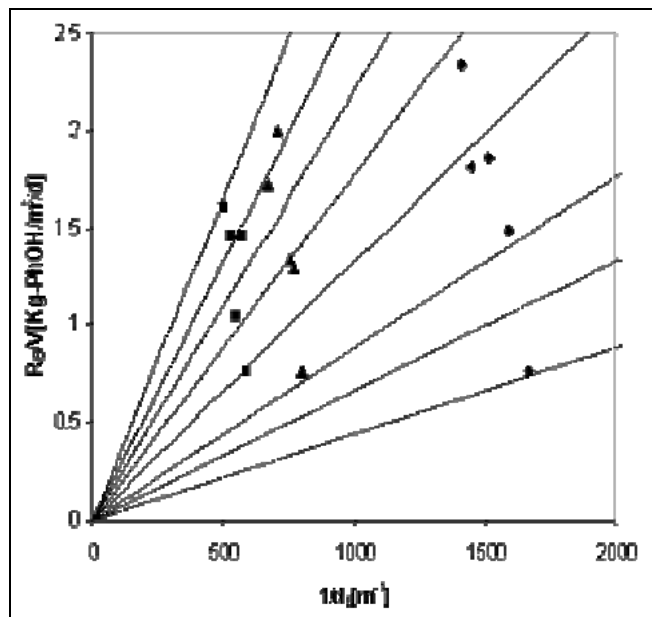
Figure 6.6: Effect of bioparticle diameter and bioparticle hold-up on phenol removal rate with biofilm

The results obtained from this research are:

- Nearly 100% of phenol removal could be achieved at a larger specific bioflim surface area per unit volumetric phenol loading rate.

- Factors that can effect the phenol removal are the specific surface area of the biofilm and the bioparticle diameter and bioparticle hold-up

From all the end pipe treatment above, the user then will select the best treatment that can be afforded by the plant in term of area needed to install cost and etc. The user can discussed further with the supplier and top management.

CHAPTER 7

CONCLUSION

Inherent Environmental Protection Analysis (IEPA) is a methodology to help the engineer or process designer to design environmental friendly process. In IEPA, the user will minimize the waste, effluent and air pollution earlier in the design stage. This IEPA analysis tool is a Microsoft Excel tool and used HYSYS as a platform to design the process. Where the data from HYSYS simulation will be export to the Microsoft Excel. Then it will be further evaluated for environment analysis in the spreadsheet.

Differ with other available methodology, IEPA applied inherent safety method and waste minimization plan its approach. There are 4 approaches in IEPA which are:

1. Substitution

   - Users have to substitute hazardous chemical with less hazardous substance. List of less hazardous substances are give in IEPA tool to help the user to implement it

2. Minimization

   - Minimization approach use chemical reaction engineering elements to help the user to minimize the volume use in the process in order to achieve the environmental requirements.

3. Moderation

   - In moderation, the IEPA tool also uses chemical engineering elements. The tool will then give some recommendations to the user on the design scheme (for this project the author scope of study is limited to reactor design scheme)

4. Limits effect

- Limit of effect is the last approach in this methodology. It will be used if all of others approaches cannot be applied. Where in limits of effect approach, the end-of-pipe treatment will be utilize. The tools will give some initiative to the user on treatment that can be applied to treat the specific chemical

The results from the case study show that the approaches can be employed to the process plant design methodology in order to overcome the environmental issue and on the same time benefits from it. There are many benefits from minimizing waste in the process which are saved money for cost, increased work and plant safety and improved product quality.

Hopefully the IEPA tool and methodology can help the engineer and process designer to take into consideration the environmental issue in the earlier design stage. By that, the environmental issue and problem that have been discussed globally will be reduced Moreover it also can promote the uses of inherent safety in the workplace.

CHAPTER 8

RECOMMENDATION

As this IEPA tool is a new developed tool, there are some recommendations that can be further expand in the future to make the tool more users friendly and integrated. Below are some of the recommendations:

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8.1   Complete other type of environmental issue evaluation

The author has divided the pollutants into 3 major parts which are effluent, waste and air pollution. In effluent, it can be further divide into 2 points which are chemical effluents and waste water. Currently, the author has covered the environmental issue for chemical effluent part.

So in future, further analysis should be done for waste and air pollution in order to complete the whole set of environmental issue.

8.2   Add the cost calculation

Furthermore, an economic potential analysis should be added to this tool so that it can help the user on the decision making steps. By showing the economic potential analysis, it can give stronger evidence to the user to apply the recommendation by the tool to their design.

8.3   Upgrade on substitution approach

In substitution approach, at present the tool have a list of 24 possible safer alterative chemical. Hopefully there will be more can be added in the future. On top of that, in this approach the author also *link* the user to the Green Chemistry Expert System (GCES) done by Environment Protection Agency (EPA) for more greener chemical and solvents

that can be sued in the process. So in the future, this GCES database can be done as HYSIS-EXCEL-GCES interface tool.

link here means that the user also needs to install the GCES in order to use the database. The GCES database comes separately with IEPA tools.

8.4   Type of reaction for moderation approach for chemical effluent

There are many types of reaction in the process. The types of reaction are:

1. Parallel reaction
2. Series reaction
3. Complex reaction
4. Independent reaction
5. Desired and undesired reaction

But in this project, the author limits it just for parallel reaction for one reactant and 2 reactants. Therefore, others type of reaction can be added to the tool. So further study should be done in order to make the tool more perfect and broaden.

8.5   Broaden the study to other equipment

At present, the tool is more on the analysis on reactor. Therefore, it must be broaden the study to other types of equipment such as distillation column, separator, dryer and etc.

8.6   To extend moderation approach with recycling method

At this moment, the tool only has moderation that use equation to moderate the operating parameters. So, for future study, recycling method in waste minimization concept can be added under the moderation approach.

CHAPTER 9

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CHAPTER 10

APPENDICES

Appendix A: IEPA Step to Step Instruction

Introduction

From the generic framework, the author has developed Inherent Environmental Protection Analysis (IEPA) tool. This tool is still in working progress.

Getting Started with IEPA

The tool is a spreadsheet program where the author used Microsoft Excel as the platform. The author chooses to use the Microsoft Excel because most of computer users in Malaysia have this software. The tool also will link the user with HYSIS simulator for adjustment and designing phase. Below is the main page for the tool:
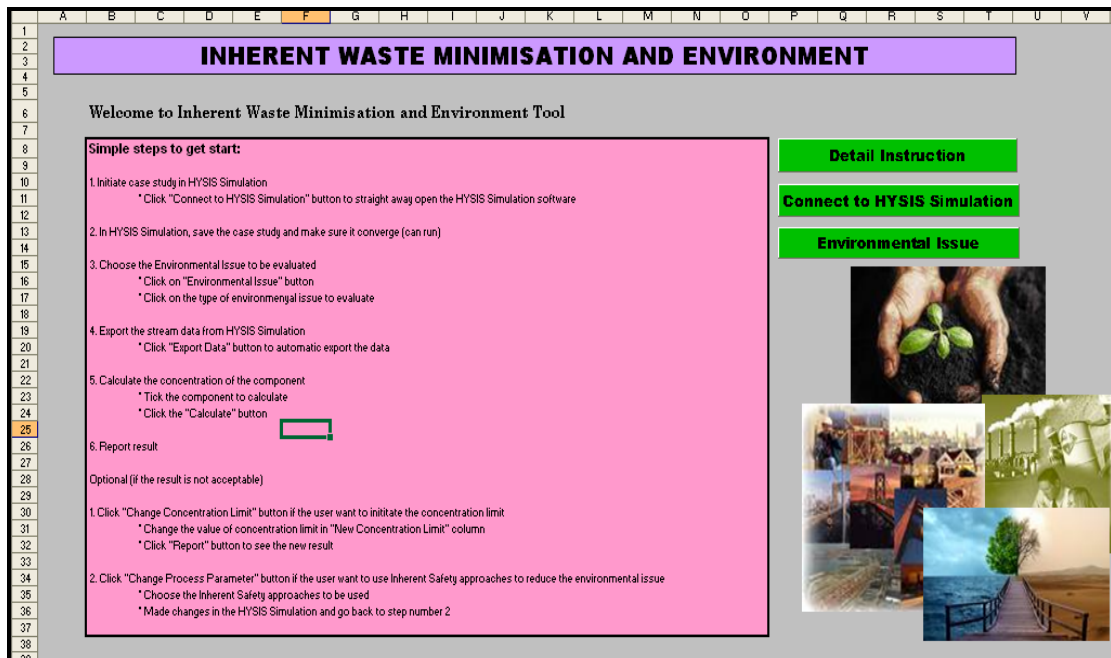
Figure 10.1: The main page of the tool

In the main page, the user will be provided a guide (step by step procedure) on how to use the tool. The details procedure is as follows:

A.1   ***Initiate case study in HYSIS Simulation***

- User need to click "Connect to HYSYS Simulation" button to straight away open the HYSYS Simulation software

A.2   ***In HYSIS Simulation, save the case study and make sure it converge***

- User need to initiate the process design and try to run the simulator to confirm that the design can be converge

A.3   ***Choose the Environmental Issue to be evaluated***

- User need to click on "Environmental Issue" button
- Then, click on the type of environmental issue to evaluate
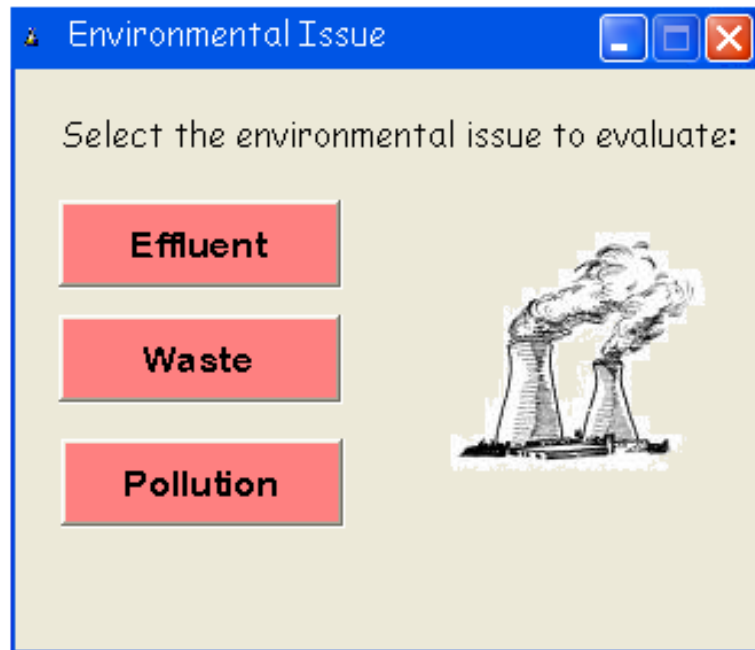
Figure 10.2: Environmental issue window

For example, the user clicks at the 'Effluent' button and choose to evaluate the chemical effluent
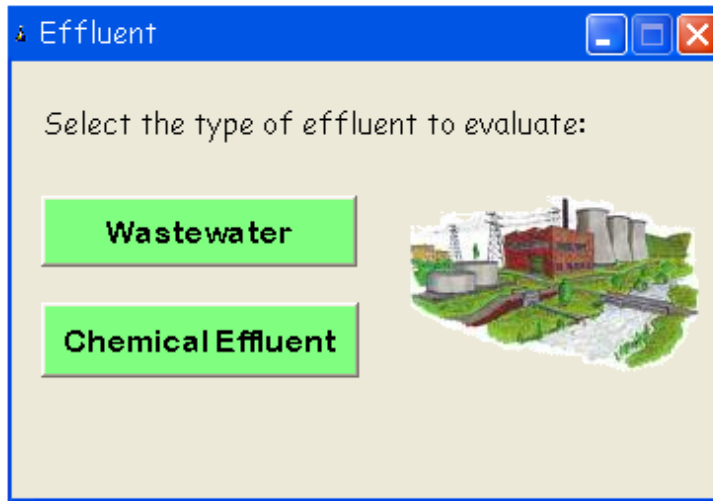
Figure 10.3: Types of issue under effluent

A.4 Export the stream data from HYSYS Simulation

▪ User need to click "Export Data" button so that the tool will automatically import the data from the HYSYS simulation
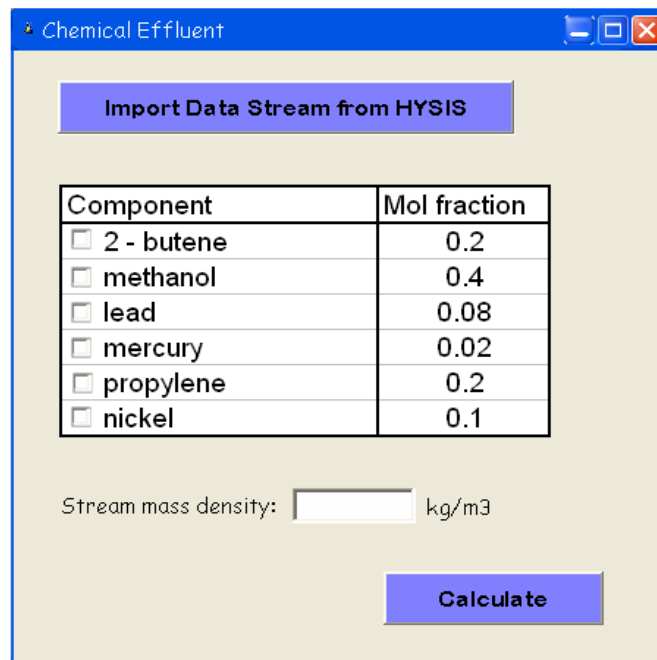
Figure 10.4 Imported data from HYSIS simulation

A.5   *Calculate the concentration of the component*

- User need to tick the component to be evaluated

- Then, click the "Calculate" button

A.6   *Report result*

- The tool will give you the report based on the concentration limit provided by EPA and Ministry of National Resources and Environment

- If the report is "Good", the user needs to continue with others environmental issue until all of them (effluent, waste and pollution) have been evaluated.

- If the report is "Exceed limit", the user need to made changes in the process parameter to have better result

Component	Concentration (mg/l)	Conc. Limit (mg/l)	Report
lead	0.13	0.1	Exceed limit
mercury	0.004	0.005	Good
nickel	0.4	0.2	Exceed limit

Change process parameter

Figure 10.5: Result window

A.7   *Changing process parameter*

- User need to choose any of the inherent safety approaches to minimize the issue for better result
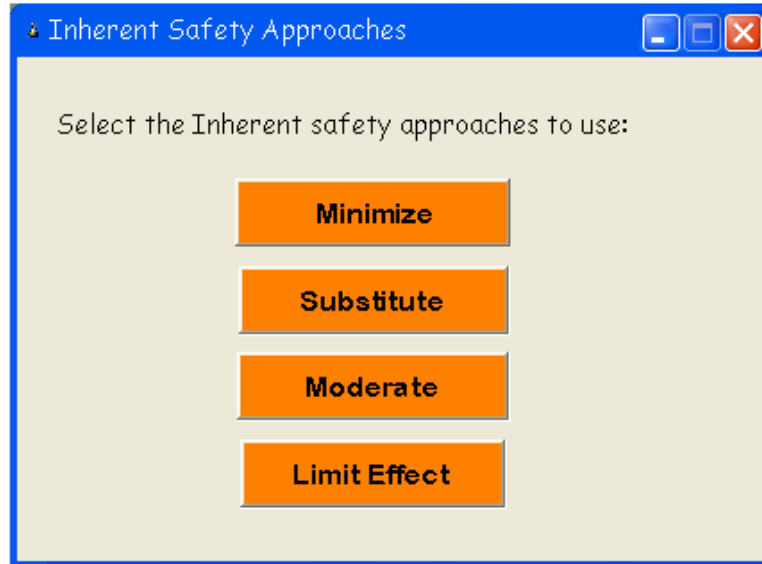
Figure 10.6: Type of inherent safety approaches that can be used for better result

Appendix B: Result from IEPA

Figure 10.7: Concentration limit calculation

ENVIRONMENTAL QUALITY (SEWAGE AND INDUSTRIAL EFFLUENTS) REGULATIONS

[Regulation 11 (5) (b)]

PARAMETER LIMITS OF EFFLUENT OTHER THAN OF STANDARD A OR B

Parameter Units Limit

(i) Temperature	°c	45
(ii) pH Value	-	5.0-9.0
(iii) BOD_5 at 20°c	mg/1	400
(iv) COD	mg/1	1000
(v) Suspended Solids	mg/1	400
(vi) Mercury	mg/1	0.10
(vii) Cadmium	mg/1	1.0
(viii) Chromium, Hexavalant	mg/1	2.0
(ix) Arsenic	mg/1	2.0
(x) Cyanide	mg/1	2.0
(xi) Lead	mg/1	2.0
(xii) Chromium, Trivalent	mg/1	10
(xiii) Copper	mg/1	10
(xiv) Manganese	mg/1	10
(xv) Nickel	mg/1	10
(xvi) Tin	mg/1	10
(xvii) Zinc	mg/1	10
(xviii) Iron (Fe)	mg/1	50
(xix) Phenol	mg/1	5.0
(xx) Sulphide	mg/1	2.0
(xxi) Oil and Grease	mg/1	100

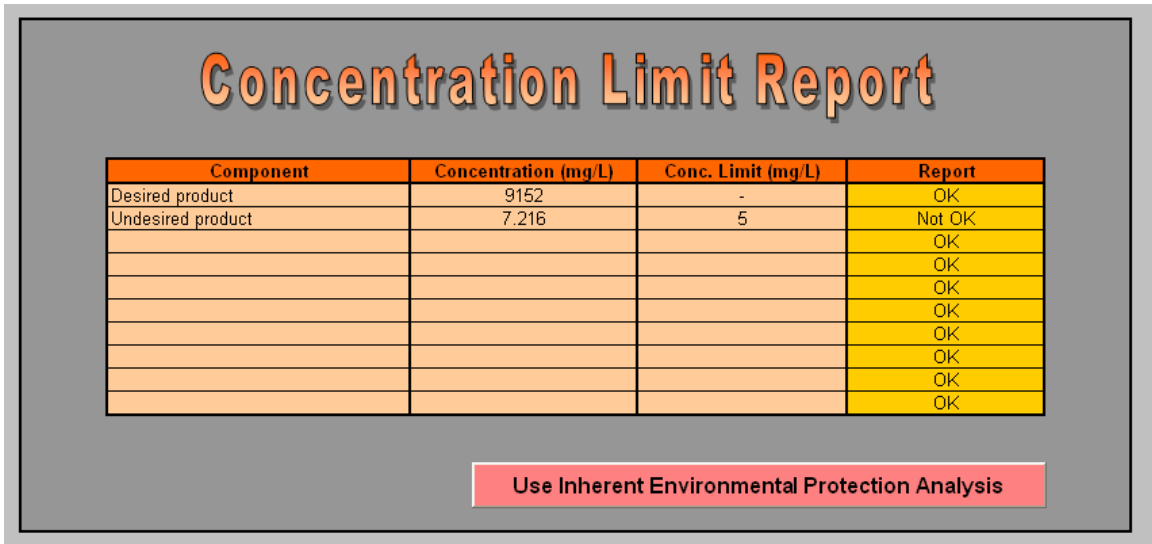Figure 10.8: Chemical concentration limit by Environment Quality Act
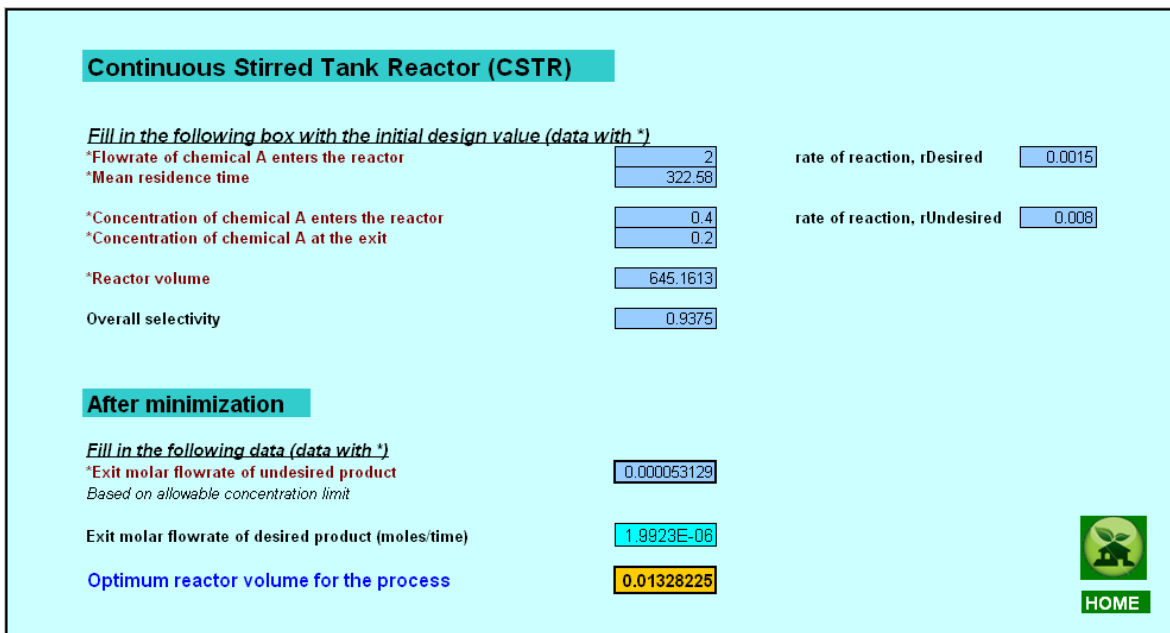
Figure 10.9: Concentration limit report

Figure 10.10: Volume minimization calculation

Figure 10.11: Moderation calculation

Figure 10.12: Moderation recommendation reactor scheme design

Table 10.1: The selectivity as a function on concentration A

Ca	S
0	#DIV/0!
0.001	187.5
0.002	93.75
0.003	62.5
0.004	46.875
0.005	37.5
0.006	31.25
0.007	26.78571
0.008	23.4375
0.009	20.83333
0.01	18.75
0.011	17.04545
0.012	15.625
0.013	14.42308
0.014	13.39286
0.015	12.5
0.016	11.71875
0.017	11.02941

The suggested outlet concentration limit is place between this range.
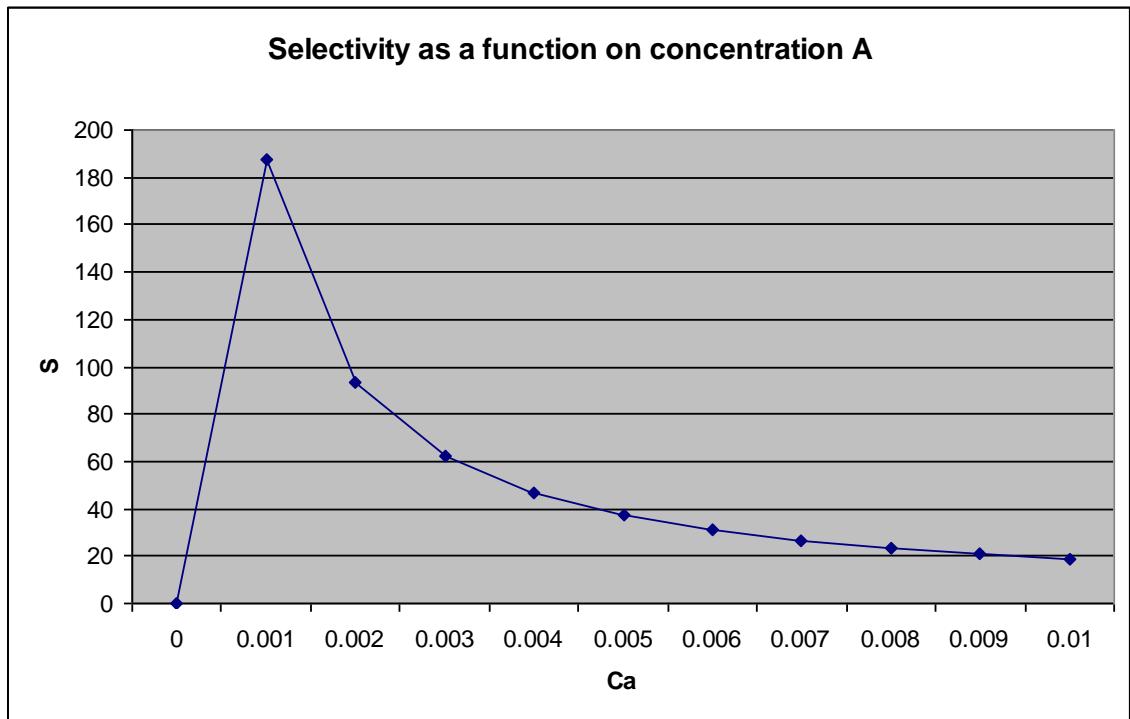

Figure 10.13: Graph selectivity as a function on concentration A in detail moderation analysis

To calculate the selectivity, user need to use the equation below

$$Selectivity = \frac{r_{desired}}{r_{undesired}}$$

*Fill all the data in the table on the right-hand side

After Moderation

Concentration limit | 5.31E-05 | Residence time | 322.58
Based on the allowable limit given

Rate constant for undesired product | 0.008 | Optimum selectivity | 41.66667

Optimum concentration outlet | 0.0045373

HOME

Figure 10.14: Detail analysis on optimum concentration outlet