# DETERMINATION OF ENERGY USAGE AND POTENTIAL ENVIRONMENT IMPACT (PEI) OF A VAPOR COMPRESSION DISTILLATION SYSTEM FOR PRODUCTION OF WATER FOR INJECTION (WFI) IN PHARMACEUTICAL INDUSTRIES

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#### **ABSTRACT**

This paper presents the potential environment impact (PEI) and energy usage studies of Water For Injection (WFI) manufacturing using vapor compression distillation (VCD) system. The amount of PEI were analysed in waste reduction (WAR) algorithm using the amount of energy usage adapted from simulation. The equations used were developed in Excel spreadsheet. There are eight impact categories were calculated to determine the effect from chemical process to the environment. Result from Excel calculation shows that Human Toxicity Potential by inhalation/dermal exposure (HTPE) has the highest value among others impact. The energy usages of VCD system were calculated by simulating the VCD process flow diagram using SuperPro Designer (SPD). The modelling result evaluate that the total energy consumption of WFI from VCD system is 53.07kWh. Since VCD system use electricity as their power supply, therefore some hazardous gases are emitted to atmosphere such as CO<sup>2</sup>, SO<sup>2</sup> and NO<sub>X</sub>. CO<sup>2</sup> has highest amount of emitted from the process with value 112.19. Result from this research may be useful to prevent the excess of CO<sup>2</sup> to our environment.

#### **ABSTRAK**

Kertas kerja ini menerangkan tentang potensi kesan terhadap alam sekitar ataupun "Potential Environmental (PEI) dankajian mengenai Impact" penggunaan tenaga dalam penghasilan "Water For Injection" (WFI) menggunakan sistem "Vapor Compression Distillaton" (VCD). Jumlah PEI telah dianalisis menggunakan algoritma "Waste Reduction" (WAR) dengan mengambil kira jumlah tenaga yang diadaptasi dalam sistem simulasi. Persamaan yang digunakan telah dibina menggunakan perisiaan "Excel". Terdapat lapan kategori bagi impak yang telah dikira untuk mengetahui kesan proses kimia terhadap alam sekitar. Keputusan daripada Excel menunjukkan bahawa potensi kesan toksik melalui pernafasan serta pendedahan pada kulit, "Human Toxicity Potential by Inhalation/ dermal exposure'" (HTPE) adalah yang paling tinggi berbanding yang lain. Penggunaan tenaga bagi sistem VCD telah dikira dengan mensimulasikan proses aliran VCD tersebut menggunakan "SuperPro Designer" (SPD). Keputusan bagi model tersebut mendapati keperluan tenaga WFI daripada sistem VCD adalah 53.07kWh. Memandangkan system VCD menggunakan elektrik sebagai sumber tenaga, beberapa gas berbahaya seperti CO2, SO2 dan NOx telah dibebaskan ke atmosfera. CO<sub>2</sub> adalah gas yang paling banyak dibebaskan daripada proses tersebut dengan nilai 112.19. Keputusan yang diperolehi daripada hasil kerja ini mungkin berguna bagi mencegah pembebasan gas CO<sub>2</sub> terhadap alam sekitar.

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# LIST OF ABBREVIATIONS

 $\hat{I}$ impact category weight

rates of PEI per unit mass of product [PEI/kg]

[Score] average value of chemical impact  $\psi^s$ specific PEI of chemical component

Mmass flowrate [kg/hr] Score value of chemical impact

mass fraction

## Subscripts

chemical component chemical mass process ср energy generate process ер gen energy generation process

h stream

impact categories i

in input output out product p total

waste energy lost we

# LIST OF ABBREVIATIONS

AP acidification potential ATP aquatic toxicity potential EP European Pharmacopoeia

GHG greenhouse gases

GWP global warming potential

HTPE human toxicity potential by inhalation/dermal exposure

HTPI human toxicity potential by ingestion

LCA life cycle analysis

ODP ozone depletion potential

PCOP photochemical oxidation (or smog formation) potential

PEI potential environment impact

SPD SuperPro designer

VCD vapor compression distillation

TLV threshold limit value

TTP terrestrial toxicity potential TWA time-weighted averages

VECs valued environmental components

VOC volatile organic compound WAR waste reduction algorithm

WFI Water For Injection

WPU water for pharmaceutical use

## 1 INTRODUCTION

## 1.1 Motivation and statement of problem

Nowadays, there were many industries that come with their own technology development from days to days and the pharmaceutical industry is one of it. General meaning for pharmaceutical industry is an industry where groups of people develop and manufacture medicine and drugs. One of the utilities they produce is Water For Injection (WFI). WFI is the highest quality of pharmacopoeia WPU and widely used in the pharmaceutical industry. WPU is water for pharmaceutical use. WFI should be used in injectable product preparations, for dissolving or diluting substances or preparations for parenteral administration before use, and sterile water for preparation of injections. No antimicrobial or other substance has been added and the pH is in between 5.0 to 7.0. In order to achieve of pharmacopoeia regulations, the WFI production process requires a higher temperature during the procedure and that led to a lot usage of energy. The higher degree of energy usage will undergo the impact to the environment and act as air pollution.

As the pharmaceutical industry expands, multinational corporations face more serious environmental problems arising from increasing global production. In many countries, there are strict Green House Gas (GHG) emission regulations and there is no doubt that soon all industries including pharmaceutical industry will be faced with increasing pressure on sustainability (Goswami & Butler, 2007). WFI is one of the pharmaceutical process utilities and it has the highest quality of pharmacopoeia standards. Distillation is the only WFI production method approved by the European Pharmacopoeia and VCD method is mostly preferred (Brush & Zoccolante, 2010). However, production of WFI consumes a lot of energy since it requires high temperature. VCD method is being used to optimize the usage of heat energy toward the system so that the energy can be recycled and not wasted. VCD plant process used electrical energy to charge up the equipments and the water in process unit. During the electricity generation process, indirectly several gases are emitted such as CO<sub>2</sub>, SO<sub>2</sub> and NO<sub>x</sub> which are hazardous. Because of arising environmental consciousness in the world today, many countries have been forced to abate the emissions, especially CO<sub>2</sub> (Mahlia, 2003). SuperPro

Designer was used to simulate the VCD process flow in order to get the value of energy usage during the process whilst the Waste reduction (WAR) algorithm method was used for assessing environment impact.

# 1.2 Objectives

The following are the objectives of this research:

 To determine the energy usage and potential environment impact of a Vapor Compression distillation system for production of Water For Injection in Pharmaceutical industries using Waste Reduction algorithm.

# 1.3 Scope of this research

The following are the scope of this research:

- i) Simulate the VCD system process flow diagram using SPD to calculate amount of energy generated per unit of time
- ii) The amount of energy generated were used to calculate the amount of each PEI indicator
- iii) The amount of each indicator was analysed using the WAR algorithm in an Excel spreadsheet

# 1.4 Main contribution of this work

The following are the contributions of this research:

- VCD process flow diagram and equation for each PEI indicator.
- Environment impact for WFI production using VCD

# 1.5 Organisation of this thesis

The structure of the reminder of the thesis is outlined as follow:

Chapter 2 provides a description of the pharmaceutical industry and the process utility which is Water For Injection. A general description of applications and general design features of vapor compression distillation system. This chapter also provides information of the energy usage and potential environment impact.

Chapter 3 gives a review of the method applied for determination of steam generated, energy usage and potential environment impact by using waste reduction algorithm. A detailed description of the algorithm used for environmental assessment is also outlined.

Chapter 4 is devoted to result and discussion for an environmental assessment, total energy demand during operation, PEI indication comparison and energy comparison between VCD with others method. All the calculations were calculated in an Excel spreadsheet with specific equation.

Chapter 5 draws together a conclusion and recommendation outlines the future work which might be derived from the model developed in this research.

## 2 LITERATURE REVIEW

## 2.1 Introduction to pharmaceutical

Malaysia External Trade Development Corporation (2011) stated that the pharmaceutical industry is an important part of the health care sector in Malaysia and high growth potential, both in domestic and export markets. Over the last decade, the Malaysian pharmaceutical market grew at between 8 to 10% annually. The market is based on a strong domestic generic sector and imports of branded and patented medicines. The potential of the domestic pharmaceutical industry has been recognized by the Malaysian government which has identified it as a strategic industry which should be promoted. One of the process utility they produce is Water For Injection (WFI).

## 2.2 Water For Injection

Water is the most frequently used as raw material in the pharmaceutical industry. Most processes require water and other ultra pure media which fulfil the legal provisions defined in pharmacopoeia. WFI is one of the pharmaceutical utilities and it is the highest quality of pharmacopoeia standards. According to a study done by Brush and Zoccolante (2010), to meet European Pharmacopoeia (EP) requirements the raw water must pass all the criteria tests before it declared as WFI. World Health Organization (2005) stated WFI is not sterile water and is not a final dosage form. It is water for the preparation of medicines for parenteral administration when water is used as vehicle (Water For Injection in bulk) and for dissolving or diluting of substances or preparations for parenteral administration (sterilised Water For Injection). Table 2.1 shows the criteria of the European Pharmacopoeia (EP) requirements.

Table 2-1: European Pharmacopoeia requirements of WFI

Water For Injection (WFI)				
Production process	Distillation			
Electrical conductivity	1.1μS/ cm (20 °C)			
Total organic carbon (TOC)	500 ppb			
Nitrate	0.2 ppm			
Heavy metals	0.1 ppm			
Colony-forming units	10 CFU/ 100ml			
Bacterial endotoxins	0.25 EU/ml			

There are several methods to produce WFI which are distillation, reverse osmosis, purification process and also ultrafiltration. Among these methods, distillation is the only WFI method of production that is approved by the European Pharmacopoeia. Brush and Zoccolante (2010) mentioned in their study that distillation has been preferred method for producing WFI in the biopharmaceutical industry, and now, most pharmaceutical WFI is produced by distillation.

# 2.3 WFI production process

The pharmaceutical industry consumes great volumes of high quality water as water for process and or in the production of medicaments (Castro et al., 2005). WFI is in priority since it is the highest quality among others WPU in pharmacopoeia standards. Distillation process or method has been chosen for production of WFI in the pharmaceutical industry. There are two processes under distillation which are multiple-effect distillation (MED) and vapor compression distillation (VCD). Vapor compression systems are based on the principle of the heat pump, with the four cycles of evaporation, compression, condensation and expansion. According to Sommer (2005), the advantage of these systems is the small amount of heat needed, although this can also be regarded as a drawback from the pharmaceutical viewpoint, since higher temperatures would provide better protection against the growth of germs in the water.

In these systems, the water is evaporated at a low pressure (in some cases in a vacuum) and at a correspondingly low temperature, and is subsequently condensed again. VCD method is being used to optimize the usage of heat energy toward the system so that energy can be recycled and not being wasted. Table 2.2 shows the overview of VCD

system..

Table 2-2: Overview VCD system

Vapor	Compression Distillation		
	The VCD needs only softened feedwater to		
Feedwater requirements	produce Water For Injection. Resulting in lower		
	pre-treatment investment and running costs.		
	The VCD does have a higher initial investment		
	cost than the MED, however the VCD can		
Time in the continuation	provide significant energy savings and a short		
Financial considerations	payback period for WFI requirements over 20		
	gpm and /or where WFI requirement is high in		
	relation to that of purified water.		
	The VCD is a rotating piece of equipment and		
Maintenance issues	therefore requires more maintenance than a		
	MED		

Vapor Compression is most preferred as the method since it is typically more energy efficient than multiple-effect distillation and also may not require a complex system design (Brush & Zoccolante, 2010). Similar finding from the study done by Hamed et al. (1996), they stated that the unique characteristic of vapor compression is the energy reuse of the vapor generated in the last effect by compressing act as a heat source for the first effect.

More suitable for larger applications, those the VCD system can be up to 3 times more efficient than other systems. The VCD offers the additional benefit of being able to utilise lower purity feedwater to produce WFI, reducing overall plant investment and maintenance issues. Figure 2-1 shows the VCD diagram adapted from Aqua-Chem (Global Water Solution).

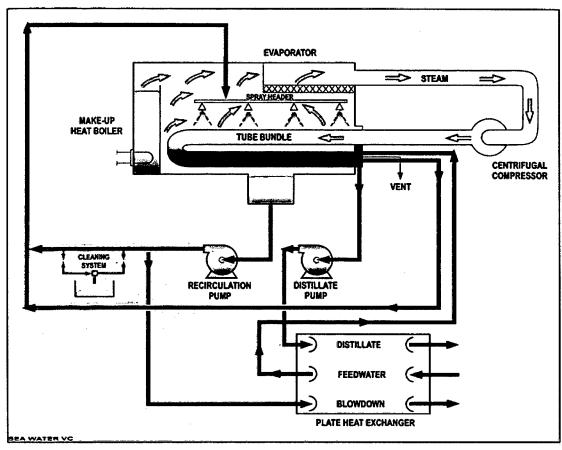


Figure 2-1: Flow diagram of VCD system

Source: Aqua-Chem (Global Water Solution)

## 2.4 Energy usage

Production of WFI consumes a lot of energy since it requires a higher temperature during the process. VCD process is using energy from the latent heat of vapor to occur in the heat transfer between vapor and liquid in the system. The energy in the system is being recycled beside of the make-up heat to maintain the optimum temperature. In Malaysia, the VCD plant process used electrical energy to charge up the equipments and heat the water in the distillation unit. According to Shekarchain et al. (2011) the electricity is generated from fossil fuel and mostly produced in combined cycle power plant. In a power plant, heat from the combustion of fossil fuel will move to generator turbine to create electricity. During the electricity generation process, several gases are emitted such as CO<sub>2</sub>, SO<sub>2</sub> and NO<sub>X</sub>. These gases are exposed to our environment and act as one of the air pollutant. The power sector contributes a significant amount of CO<sub>2</sub> emitted into the atmosphere due to burning of fossil fuels (Sin, Indati, Mustapa, & Peng, 2011).

# 2.5 Potential environment impact

Although the pharmaceutical industry is not considered a 'dirty' industry compared too many others, it faces new challenges in controlling and preventing environmental pollution as it expands (Berry & Rondinelli, 2002). According to a study done by Young & Cabezas (1999), the potential environment impact of a given quantity of material and energy can be generally defined as the effect that this material and energy would have on the environment if they were to be emitted into the environment. Gases emitted from the production process are the acidic gasses that will affect our climate and poison ground water. On the other hand, the Malaysian Government has shown serious concerns on the issues of greenhouse gases (GHG) emission, and climate change (Arshad, Ibrahim, Anuar, Shukrie, & Razak, 2012).

Heijungs et al. (1992) stated the classification of impact categories fall into two general areas of concern with four categories in each area. Table 2-3 showed the classification of impact categories The potential environmental impacts are calculated from stream mass flow rates, stream composition, and a relative potential environmental impact score for each chemical present (Cabezas, Bare, & Mallick, 1999). According to Othman (2011), an engineer of process design systems must through a careful selection of process operating conditions, since the lower the PEI value, the more desirable the process.

Table 2-3: Classification of impact categories

Global atmospheric		Local Toxicological				
Global Warming Potential (GWP)				Human Toxicity Potential By Ingestion (HTPI)		
Ozone Depletion Potential (ODP)		Human Toxicity Potential By Expose Both Dermal and Inhalation (HTPE)				
				Both Dermai and Illianation (1111E)		
Acidification or	Acid rain Pot	entia	l (AP)	Aquatic Toxicity Potential (ATP)		
Photochemical	Oxidation	or	Smog	Terrestrial Toxicity Potential (TTP)		
Formation Poten	tial (PCOP)					

Basically, every material that comes into the manufacturing process has PEI input, during the reaction (PEI generated) and total PEI exit at output stream (PEI output). Therefore, PEI input plus PEI generated equal to PEI output. For energy, PEI input did

not consider, then, during energy production generated is output. There are four main environmental indicators will calculate and evaluate from WAR algorithm;  $I_{gen}^t$ ,  $I_{out}^t$ ,  $\hat{I}_{gen}^t$  and  $\hat{I}_{out}^t$ . Here some equations use to calculate these indicators. The total rate of PEI generated,  $I_{gen}^t$  and total PEI output,  $I_{out}^t$ , can be expressed as:

$$I_{gen}^t = I_{out}^{cp} - I_{in}^{cp} + I_{out}^{ep}$$

$$I_{out}^t = I_{out}^{cp} + I_{out}^{ep}$$

The indices presented to this end are in terms of rate PEI/h. To evaluate on a product basis (PEI/kg), a simple transformation can be made to the index by,

$$\begin{split} \hat{I}_{gen}^t &= \frac{I_{out}^{cp} - I_{in}^{cp} + I_{out}^{ep}}{\sum M_p} \\ \hat{I}_{out}^t &= \frac{I_{out}^{cp} + I_{out}^{cp}}{\sum M_p} \end{split}$$

where  $M_p$  is the mass flow rate of product p.

## 2.6 Summary

The concept of producing WFI using compressed steam VCD dates back to the post World War era. The idea is simple by use steam to produce a purified steam, and then re-compress that steam to be used to create more purified steam, after that condensing the steam during that process into WFI. VCD is typically more energy efficient and can create ambient WFI at the lowest over-all cost.

## 3 PROCESS MODELLING AND SIMULATION

#### 3.1 Overview

This research intends to determine the energy usage and potential environment impact in the production of Water For Injection by using WAR algorithm. Thus, this research SuperPro designer is use to simulate the vapor compression process flow diagram in order to get the value of energy usage during the process. There are several methods used for determination of environment assess such as Ecoindicator 99, Product environmental life cycle analysis (LCA), Waste reduction (WAR) and also Valued Environmental Components (VECs). Nevertheless, this research focus to perform environmental analysis for the production of Water For Injection (WFI) using vapor compression system for pharmaceutical use based on Waste reduction (WAR) algorithm. So far, there is no current research focusing on evaluation of environmental performance for WFI.

## 3.2 Environmental assessment using WAR algorithm

According to Young & Cabezas (1999) the WAR algorithm is a methodology used for determining the PEI of a chemical process. WAR algorithm does not represent a complete life cycle analysis (LCA) and it is simply a tool to be used by the design engineer to aid in evaluating the environmental friendliness of a process. The researcher also stated that only electrical energy is considered in the calculation of PEI.

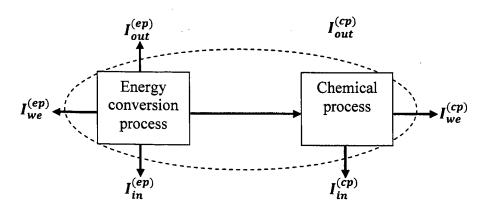


Figure 3-1: Mass and energy balance for the calculation of the PEI at the manufacturing level.

The figure 3-1 shows the mass and energy balance for the calculation of PEI at the manufacturing level and Othman (2011) mentioned in his research that the concept of PEI in the WAR algorithm is based on the conventional mass and energy. The key formulations of the algorithm are briefly reviewed below.

At the steady state, the algorithm can be expressed as:

$$I_{in}^{cp} + I_{in}^{ep} - I_{out}^{cp} - I_{out}^{ep} - I_{we}^{cp} - I_{we}^{ep} + I_{gen}^{t} = 0$$

where  $I_{in}^{cp}$  and  $I_{out}^{cp}$  are, respectively, mass input and output rates of PEI of a chemical process:  $I_{in}^{ep}$  and  $I_{out}^{ep}$  are, respective;y, the energy input and output rates of PEI of the energy conversion process;  $I_{we}^{cp}$  and  $I_{we}^{ep}$  are, respectively, the outputs of PEI associated with waste energy lost from the chemical process and the energy conversion process;  $I_{gen}^{t}$  is the total rate of energy of PEI inside the system, representing the creation and consumption of PEI by chemical reactions. Young & Cabezas has stated in their research that  $I_{we}^{cp}$  and  $I_{we}^{ep}$  can be ignored because chemical plants usually do not emit large amounts of waste energy and the PEI of mass is much greater than the emission of energy.

Hence, the equation at steady can be simplified as,

$$I_{aen}^t = I_{out}^{cp} - I_{in}^{cp} + I_{out}^{ep} - I_{in}^{ep}$$

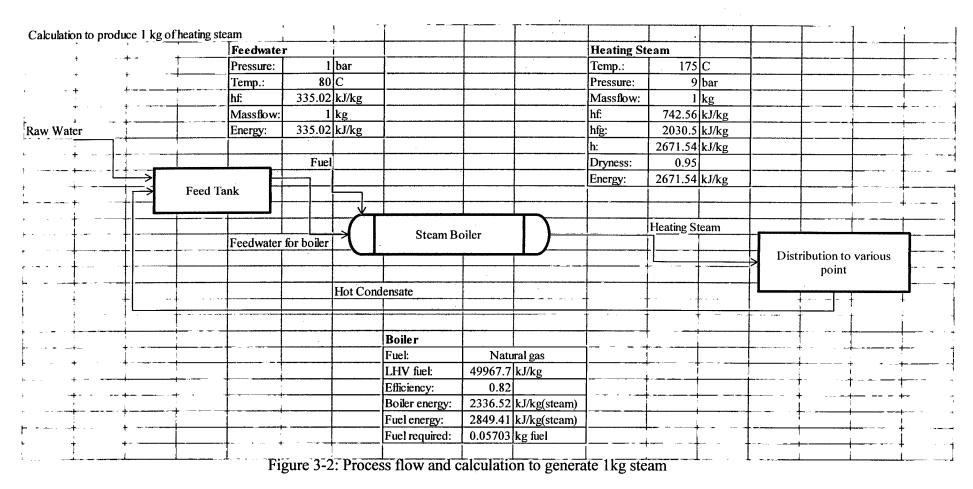
Equation for I<sub>in</sub><sup>cp</sup> and I<sub>out</sub><sup>cp</sup> can be expressed as:

$$I_{in}^{cp} = \sum_{h}^{Streams} \sum_{c}^{Comps} M_{h,in} \sum_{c}^{Comp} (x_{c,h} \psi_{c,i}^{s})$$
 and 
$$I_{out}^{cp} = \sum_{h}^{Streams} \sum_{c}^{Comps} M_{h,out} \sum_{c}^{Comp} (x_{c,h} \psi_{c,i}^{s})$$

where  $M_h$  is the mass flow rate of the stream h, either input or output stream;  $x_{c,h}$  is the mass fraction of component c in stream h;  $\psi^s_{c,i}$  is specific PEI of chemical c for impact category i.

## 3.3 Energy usage to generate steam

A process flow diagram to generate steam and Figure 3-2 shows the calculation to produce 1 kg of heating steam by using Excel spreadsheet whereas Table 3-1 shows the heat transfer agent (steam) demand for VCD process.



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Table 3-1: Heat transfer agent demand

1.1b Heat transfer Agent Demand				
Steam	kg/yr	kg/h	kg/kgMP	
Main Section	786823.2	89.82	N/A	
TOTAL	786823.2	89.82	N/A	

Source: Adapted from SPD result under Utilities & Labor report.

The calculation for lower heating value (LHV) can be reviewed at Appendices.

## 3.4 Specific PEI of chemical components

According to research done by Heijungs et al. (1992), the impact categories to determine the affect from chemical process to the environment is generally classified into two main categories. The main categories are global atmospheric and local toxilogical. The calculation of  $\psi^s$  is based on scores using the equation below:

$$\beta_i \psi^s_{c,i} = \frac{score_{c,i}}{[score_c]_i}$$

where  $\beta_i$  represents the relative weighting factor of impact categories i that should be used to emphasize or de-emphasize specific impact categories. Score<sub>c,i</sub> represents the value of chemical c on some arbitrary scale for impact category i and [Score<sub>c</sub>]<sub>i</sub> represents the average value of all chemicals in category i.

Table 3-2 below shows the method to determine all the impact categories and Table 3-3 shows the four main environmental indicators that will be calculated and evaluate their value. All the data adapted from Othman (2011) and Heijungs et al. (1992).

Table 3-2: Method to determine all the impact categories

Impact Categories	Method
	Comparing the extent to which a unit mass of
Global Warming Potential (GWP)	a chemical absorbs infrared radiation over its
	atmospheric lifetime to the extent that CO <sub>2</sub>
	absorbs infrared radiation over its respective
	lifetimes.
Ozone Depletion Potential (ODP)	Comparing the rate at which a unit mass of
	chemical reacts with ozone to form

molecular oxygen to the rate at which a unit mass of CFC-11 (trichlorouoromethane) reacts with ozone to form molecular oxygen.  Comparing the rate of release of H+ in the atmosphere as promoted by a chemical to the rate of release of H+ in the atmosphere as promoted by SO <sub>2</sub> .  Photochemical Oxidation or Smog Formation Potential (PCOP)  Comparing the rate at which a unit mass of chemical reacts with a hydroxyl radical (OH) to the rate at which a unit mass of ethylene reacts with OH.  Estimate the value using lethal dose, LD50  Ingestion (HTPI)  Estimate the value using time-weighted
reacts with ozone to form molecular oxygen.  Comparing the rate of release of H+ in the atmosphere as promoted by a chemical to the rate of release of H+ in the atmosphere as promoted by SO <sub>2</sub> .  Photochemical Oxidation or Smog Formation Potential (PCOP)  Comparing the rate of release of H+ in the atmosphere as promoted by SO <sub>2</sub> .  Comparing the rate at which a unit mass of chemical reacts with a hydroxyl radical (OH) to the rate at which a unit mass of ethylene reacts with OH.  Human Toxicity Potential By  Ingestion (HTPI)  Estimate the value using lethal dose, LD50
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Ingestion (HTPI)  Estimate the value using time-weighted
Estimate the value using time-weighted
Estimate the value using time-weighted
Human Toxicity Potential By Expose averages (TWA) of the threshold limit values
Both Dermal and Inhalation (HTPE) (TLV)
Aquatic Toxicity Potential (ATP) Estimate the value using lethal concentration,
LC50
Terrestrial Toxicity Potential (TTP) Estimate the value using lethal dose, LD50

Table 3-3: Four main environmental indicators

Environmental Indicators	Meaning
ıt rcp rcp rep	Useful in comparing processes based on the amount
$I_{\text{gen}}^{\text{t}} = I_{\text{out}}^{\text{cp}} - I_{\text{in}}^{\text{cp}} + I_{\text{out}}^{\text{ep}}$	of new PEI generated in product manufacturing.
$I_{\text{out}}^{\text{t}} = I_{\text{out}}^{\text{cp}} + I_{\text{out}}^{\text{ep}}$	To identify an appropriate site for a plant.
$\hat{I}_{gen}^{t} = \frac{I_{out}^{cp} - I_{in}^{cp} + I_{out}^{ep}}{\sum M_{p}}$	Used for comparing processes and products based on
$\sum M_p$	the amount of new potential environmental impact
	generated in product manufacturing.
$\hat{I}_{out}^{t} = \frac{I_{out}^{cp} + I_{out}^{cp}}{\sum M_{p}}$	Measures the efficiency of material utilization by a
$\Sigma M_{ m p}$	specific process per unit mass of products

where  $M_p$  is the mass flow rate of product p.

According to a research by Othman (2011) a chemical when the value increase or higher the toxicity will decrease or lower and for WAR algorithm, when the score higher the potential environmental impact also higher. The score for chemical c for HTPI and TTP can be measured by:

$$Score_{c,HTPI,TTP} = (LD 50)_c^{-1}$$

whereas for ATP:

$$Score_{c,ATP} = (LC 50)_c^{-1}$$

Table 3-4 till Table 3-6 shows the PEI calculation and it is developed in excel spreadsheet whereas Table 3-7 shows the emission factor and specific PEI of component from energy consumption.

Table 3-4: Impact factor (energy) with hazardous gases value for each PEI indicator

Gases	SOx	NOx	CO	CO
Component	SOX	NOX	$CO_2$	CO
HTPI	1.2	0.78	0	0
HTPE	0	5.6	9000	29
ATP	0	1.96	0	0
TTP	1.2	0.78	0	: 0
GWP	0	0	1	0
PCOP	0	0	0	0
AP	1	1.77	0	0
ODP	0	0	0	0

Table 3-5: Specific PEI value calculation

Gases	SO	NO-	60	00
Component	SOx	NOx	$CO_2$	CO
HTPI	0.8333333	1.2820513	0	0
HTPE	0	5.6	9000	29
ATP	0	0.0510204	0	0
TTP	0.8333333	1.2820513	0	0
GWP	0	0	1	0
PCOP	0	0	0	0
AP	1	1.77	0	0
ODP	0	0	0	0

Table 3-6: Normalized PEI value from energy consumption

Gases	SOx	NOx	$CO_2$	CO
Component	30x	NOX	CO <sub>2</sub>	
HTPI	0.787878	1.2121212	0	0
HTPE	0	0.0018595	2.988511	0.009629
ATP	0	0.0510204	0	0
TTP	0.787878	1.2121212	0	0
GWP	0	0	1	0
PCOP	0	0	0	0
AP	0.722022	1.277978	0	0
ODP	0	0	0	0

Table 3-7: Emission factor and specific PEI of component from energy consumption

Component	Emission Factor (kg/kWh)	Specific PEI of component
$SO_X$	0.0005	0.51
$NO_{X}$	0.0009	1.88
$CO_2$	0.53	938.93
CO	0.0005	0.00

# 3.5 SuperPro designer

One of the technologies to produce WFI is VCD. Simulation of VCD will be done by using Super Pro software. Super Pro software or designer includes a variety of unit operations models treatment and purification of air and gaseous streams in general. This software can be used to calculate emissions of volatile organic compounds (VOCs) from batch chemical manufacturing operations, design and evaluate in a cost effective way pollution control technologies that meet regulatory standards. Amount of energy usage from WFI production can be calculated by using Super Pro software.

After the value of energy usage was calculated, the value was used to find potential environmental impact (PEI) using WAR algorithm. Report from simulation can be reviewed at the appendices.